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NSRDS-NBS 72

U.S. DEPARTMENT OF COMMERCE / National Bureau of Standards

Tables of Rate Constants for Gas Phase Chemical Reactions of Sulfur Compounds (1971-1980)

QC
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.U573
No.72
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Tables of Rate Constants for Gas Phase Chemical Reactions of Sulfur Compounds (1971-1980)

NSRDS-NBS

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U.S. DEPARTMENT OF COMMERCE, Malcolm Baldrige, Secretary
NATIONAL BUREAU OF STANDARDS, Ernest Ambler, Director

Issued May 1982

Library of Congress Cataloging in Publication Data

Westley, Francis
Tables of rate constants for gas phase chemical reactions of sulfur compounds (1971-1980)

(NSRDS-NBS ; 72)
"Issued May 1982."
1. Chemical reaction, Rate of—Tables. 2. Sulphur compounds—Tables. I. Morgantown Energy Technology Center. II. United States. National Bureau of Standards. Office of Standard Reference Data. III. Title. IV. Series.
QC100.U573 no. 72 [QD502] 602'.18s 82-2094

[546'.7232] AACR2

NSRDS-NBS 72
Nat. Stand. Ref. Data Ser., Nat. Bur. Stand. (U.S.), 72, 42 pages (May 1982)
CODEN: NSRDAP

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U.S. GOVERNMENT PRINTING OFFICE
WASHINGTON: 1982

Foreword

The National Standard Reference Data System provides access to the quantitative data of physical science, critically evaluated and compiled for convenience and readily accessible through a variety of distribution channels. The System was established in 1963 by action of the President's Office of Science and Technology and the Federal Council for Science and Technology, and responsibility to administer it was assigned to the National Bureau of Standards.

NSRDS receives advice and planning assistance from a Review Committee of the National Research Council of the National Academy of Sciences-National Academy of Engineering. A number of Advisory Panels, each concerned with a single technical area, meet regularly to examine major portions of the program, assign relative priorities, and identify specific key problems in need of further attention. For selected specific topics, the Advisory Panels sponsor subpanels which make detailed studies of users' needs, the present state of knowledge, and existing data resources as a basis for recommending one or more data compilation activities. This assembly of advisory services contributes greatly to the guidance of NSRDS activities.

The System now includes a complex of data centers and other activities in academic institutions and other laboratories. Components of the NSRDS produce compilations of critically evaluated data, reviews of the state of quantitative knowledge in specialized areas, and computations of useful functions derived from standard reference data. The centers and projects also establish criteria for evaluation and compilation of data and recommend improvements in experimental techniques. They are normally associated with research in the relevant field.

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Reliable data on the properties of matter and materials are a major foundation of scientific and technical progress. Such important activities as basic scientific research, industrial quality control, development of new materials for building and other technologies, measuring and correcting environmental pollution depend on quality reference data. In NSRDS, the Bureau's responsibility to support American science, industry, and commerce is vitally fulfilled.

ERNEST AMBLER, *Director*

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Tables of Rate Constants for Gas Phase Chemical Reactions of Sulfur Compounds (1971–1980)

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A table of rate constants for gas phase chemical reactions of sulfur compounds is presented. Specifically, it gives in tabular form the values of the parameters for the modified Arrhenius equation $k = AT^{B}\exp(-E/RT)$. The table covers the reactions of sulfur containing molecules and free radicals, S, S_2, SO, SO_2, SO_3, S_2O, SH, H_2S, CS, CS_2, COS, $CH_3S\cdot$, CH_3SH, cy-CH_2CH_2S, $CH_3SCH_2\cdot$, and a number of thiols, thioethers, and thioesters, with other compounds. The table includes 19 unimolecular, 208 bimolecular, and 13 termolecular reactions totaling 240 distinct chemical reactions. There are 441 rate constants associated with these reactions, distributed as follows: 30 for first order reactions, 377 for second order reactions, and 34 for third order reactions. The kinetic data were compiled from 145 experimental papers and 8 critical reviews published between 1971 and 1980.

Key words: Arrhenius parameters; chemical kinetics; combustion; decomposition; free radicals; gas phase; hydrocarbons; hydrogen; nitrogen; oxygen; rate of reaction; sulfur.

1. Introduction

This publication consists of a table of rate constants for reactions of inorganic and organic sulfur compounds in the gas phase, as well as of their reactions with other substrates. The table is a compilation of rate constants given in 145 experimental papers and 8 critical reviews published between 1971 and 1980. Its purpose is to provide the kineticist and combustion modeler with a comprehensive and easy-to-use source of kinetic data for chemical processes involving sulfur compounds. The table gives 441 distinct reaction rate constants from the above mentioned sources. A list of references including the 153 papers, arranged alphabetically by author for each separate year, is appended at the end of the table.

The table includes a limited number of reactions involving excited states like $S^*(^1D)$ and SO_2^*; however, no attempt was made to cover all the papers from the literature dealing with such excited species. The reader interested in the reaction kinetics of electronically excited species is encouraged to consult Keith Schofield's excellent review: "Critically Evaluated Rate Constants for Gaseous Reactions of Several Electronically Excited Species," J. Phys. Chem. Ref. Data **8**, 723 (1979).

For ease of reference the sulfur-containing reactant in a bimolecular or termolecular reaction is always placed first, so that a grouping of the reactions according to the standard order of sulfur compounds is obtained. However, 18 bimolecular reactions and 1 termolecular reaction involve 2 sulfur-containing reactants. For that reason, these 19 reactions are listed twice, the second time with the order of the sulfur-containing reactants reversed, e.g., $COS + S \rightarrow CO + S_2$ is also listed as $S + COS \rightarrow S_2 + CO$. As a result, the total number of tabulated entries is 460, although the real number of distinct entries is only 441. The arrangement of the tables and the standard order of chemical compounds are described in detail in the next section "Guidelines for the User."

The presentation of kinetic data is standardized and simplified as much as possible. Rate constants are expressed in terms of the modified Arrhenius equation $k = AT^{B}\exp(-E/RT)$. In general, uncertainties are given only for the rate constant k itself and not for the individual parameters in this equation. Sometimes an uncertainty is given for the value E/R and has been included in the uncertainty stated for the value of the rate constant. Rate constants are expressed in units of s^{-1}, $cm^3mol^{-1}s^{-1}$, and $cm^6mol^{-2}s^{-1}$ for reactions of first, second, and third order, respectively. Conversion tables for other units are appended at the end of this publication.

This publication is not the result of the effort of a single person, but of the whole staff of the Chemical Kinetics Division. My thanks go to all of them. In particular, I wish to thank Dr. Robert F. Hampson, Jr., Director of the Chemical Kinetics Data Center, for his more than helpful suggestions and constant guidance; Dr. John T. Herron, Chief of the

Chemical Kinetics Division, and Dr. Wing Tsang, of the Chemical Kinetics Division, for their encouragement; Dr. Bert R. Staples, Manager of the Electrolyte Data Center, for assistance in computer formatting; Mrs. Bettijoyce Molino and Mrs. Carla G. Messina from the Office of Standard Reference Data for applying the OMNIDATA and GPSDIC programs to photocompose the present tables; Mrs. Janice L. Jones for typing the original text with particular care; and Mrs. Miriam Oland from the Technical Information and Publications Division for retyping the text for photocomposition.

2. Guidelines for the User

General

As pointed out above, the presentation of the kinetic data in this publication is an attempt to simplify and standardize them. Units for rate constants used in this table are the cubic centimeter, the mole, and the second. The uncertainties given in this table are derived from the error limits specified by the author of the original paper or critical review. These have heen converted to a standard format, as described below. In the present tables the concern is with the overall uncertainty of a reaction rate constant and not with the expression of precision of a set of experimental measurements. Most of the uncertainty limits included in this table are uniform within the temperature range indicated. However, for a limited number of reactions, the data warrant or require variable limits. In such cases, a note under the respective data indicates for which interval of the temperature range there is a change in the uncertainty limits.

Uncertainty limits expressed in the form of lower and upper k factors, f and F, respectively, are used in this tabulation. Thus, if k_0 is the central value of a rate constant the limits of reliability for the rate constant k_0 are defined by the relationship:

$$fk_0 < k < Fk_0 \qquad (1)$$

i.e., multiplication of the central value k_0 by f and F gives, respectively, the lower and upper reliability limits of the rate constant. In this standardized formulation of uncertainty limits, the value of f is less than unity and the value of F is greater than unity.

However the k factors are not the only way to express the uncertainty limits of a rate constant and different authors use different forms to indicate the degree of reliability of a recommended rate constant. It follows that certain mathematical relationships are needed to translate the different forms of uncertainty limits into the standard form used in this table (lower and upper k factors). The formulas used to transform any form of uncertainty limits into the standard form were given and discussed at length in the introduction of a previous publication[1] and will not be repeated here.

[1] Westley, Francis, "Tables of Recommended Rate Constants for Chemical Reactions Occurring in Combustion," NBSIR 79-1941 (1979) (1st ed.); NSRDS-NBS 67 (1980) (2d ed.).

Arrangement of the Table

The table arranged in nine columns gives the chemical reaction, the order of reaction n, the "third body" collision partner M, the rate constants ratio k/k_{ref}, the temperature range in kelvins, the parameters A, B, and E/R for the modified Arrhenius equation $k = AT^{n}\exp(-E/RT)$, and the uncertainty limits expressed as k factors f and F.

The bibliography includes the full references for the 145 experimental papers and 8 critical reviews from which the present table was compiled. Following the bibliography, two conversion tables for equivalent second and third order rate constant units are appended.

The arrangement of the table is as follows:

Column 1, the chemical reaction indicating hoth the reactants and the products. In the same column, under each chemical reaction, the names of the reactants are given. The chemical nomenclature adopted is the one used in the Chemical Substance Indexes of Chemical Abstracts. Alternative names are not given. The chemical names of the products are not given. The line with chemical names is indented with respect to the line above it. Under the chemical names, the short reference to the reviewer's book or article is given. It includes the last two digits of the year of the publication followed by the first three letters of the author's name. If two authors are given, a slash separates the first three letters of each author's name. Again, the short reference line is indented with respect to the line above it, e.g., 78 MAR/HER indicates the experimental rate constant for the reaction between dimethyl sulfide and ozone, published by Martinez and Herron in 1978.

Recommended values for rate constants or ratios are indicated in parentheses after the short reference, e.g., 76 BAU/DRY (Recommended k); 72 KER/PAR (Recommended ratio).

The last line of column 1, placed under the line including the short reference, is given only when necessary and might include information about the dependence of k factors on temperature range, or the reaction taken as reference when a value for the ratio k/k_{ref} is given in column 3, or other information pertinent to the reaction indicated above. For a couple of reactions taken from Baulch et al. (76 BAU/DRY) the relationship $k_1 = Kk_{-1}$ included in the note indicates that the rate constant was calculated from the equilibrium constant K and the rate constant k_{-1} of the reverse reaction. In such cases, the author usually gives the rate constant of the reverse reaction immediately after the data for the forward reaction. The arrangement of the present table based on the standard order, does not allow the forward rate constant of a reaction to be followed immediately by its reverse rate constant. The reader will have to locate the rate constant of a reverse in its proper place in the table.

Column 2, with the heading n, indicates the order of the reaction displayed in column 1. The value of n is 1, 2, or 3, which defines the proper standard units for the reactions, as follows:

1	for the first order reactions	s^{-1}
2	for the second order reactions	$cm^3mol^{-1}s^{-1}$
3	for third order reactions	$cm^6mol^{-2}s^{-1}$

The reaction order is indicated for every reaction included in the table and the digit indicating its value is alined with the short reference.

Column 3, with the heading M, defines the inert reaction partner ("third body") when the chemical reaction displayed in column 1 includes the letter M. Most of the third bodies displayed in column 3 include no more than three characters, e.g., Ar, He, H_2O, N_2, N_2O, SO_2, SO_3, CO_2. For the reaction $SO_2 + OH + M \rightarrow HOSO_2 + M$, the third body, a mixture of N_2 and O_2, is indicated in the note in column 1. No indication is given if M is undefined in the paper. When displayed, the third body is alined with the short reference and the reaction order.

Column 4, with the heading k/k_{ref}, gives the ratio of the rate constant of the reaction indicated in column 1 and the rate constant of a reference reaction. In most cases this ratio is a dimensionless number. However, when the order of the reaction indicated in column 1 is different from the order of the reference reaction, the ratio of the rate constants is no longer dimensionless and the expression for the ratio of rate constants is not given in column 3 (for lack of space), but in the note at the end of column 1. The reference reaction is always indicated in the notes. The dimensionless rate ratios given in column 3 are alined with the short reference given in column 1 and with the reaction order given in column 2.

Column 5, with the heading T/K, gives the temperature range of validity for the corresponding rate parameters. For some reactions only one temperature is given, meaning that the reaction was studied only at one temperature. If no temperature is indicated, it means that the kinetic parameters of the corresponding reaction are valid throughout. The data estimated by Benson and Golden in their report "Estimating the Kinetics of Combustion" (75 BEN/GOL) are in this category. The temperatures are alined with the short references given in column 1, as well as with the reaction order given in column 2.

Column 6, with the heading A, gives the value of A for the equation $k = AT^B\exp(-E/RT)$. A is expressed as a number less than 10 followed by the exponent in parentheses, e.g., 3.5 (+14) should be read as $3.5 \times 10^{+14}$. The coefficient of the A factor has no more than one digit after the decimal point. The units of the A factor are the same as for the rate constant. For those cases when the recommended value is only for one temperature, the entry under this column is in fact the value of the rate constant k at this temperature. The data for the A factor are alined with the short reference and reaction order information. If a dash appears in this column, it means that no A factor value was reported by the evaluator for the corresponding reaction. In such a case a rate ratio is given in column 4.

Column 7, with the heading B, gives the value of B for the equation $k = AT^B\exp(-E/RT)$. The value of B usually lies between 0 and 4, negative or positive. No more than one digit is given after the decimal dot. A dash in this column means that no B value was reported by the evaluator. The data for B are alined with the short reference and reaction order information.

Column 8, with the heading E/R, indicates the value of E/R for the equation $k = AT^B\exp(-E/RT)$. Since E is the activation energy in cal mol^{-1} and R the gas constant with a value of 1.987 cal mol^{-1} K^{-1}, it follows that the units of E/R are kelvins. The values given in column 5 for E/R may vary from 0 to over 100,000 kelvins. The E/R values may be positive or negative. Some of the E/R values included in the table are followed by an uncertainty with plus or minus signs. As pointed out in the introduction, these uncertainties may be ignored, as they are included in the lower and upper k factors indicated in the right column of the table. A dash in this column means that no E/R value was reported by the evaluator. The values for the E/R factor are alined with the short reference and reaction order information.

Column 9, with the heading "k factors" and two subheadings, "f" and "F," indicates the two uncertainty k factors, the lower factor f in the left subcolumn and the upper factor F in the right subcolumn. To find the uncertainty limits of a reaction, its rate constant is to be multiplied by the two factors, as shown in (1): $fk_0 < k < Fk_0$. The values of both factors are always positive. If no uncertainty limits are indicated by the evaluator, both subcolumns of the column 6 are left blank. The k factors are alined with the short reference and reaction order information.

Ordering of Chemical Reactions

The general rule for ordering the chemical reactions listed in column 1 of the table is the standard order of arrangement as described in NBS Technical Note 270-3.[2] A detailed discussion of this rule was presented in the introduction to the publication noted in the preceding footnote (NBSIR 79-1941/1979, or NSRDS-NBS 67/1980) and will not be repeated here. It suffices to say that this rule is applied to the first reactants of the reactions listed in this table, as well as to the reactants following the first, and that the first reactant of a reaction takes precedence over the following ones. The compounds listed in the Contents, which give only the first reactants of the chemical reactions included in this work, are in the standard order (S, S_2, SO, SO_2, SO_3, S_2O, SH, H_2S, CS, CS_2, COS, CH_3S·, cy-CH_2CH_2S, etc.) and are each part of the S–O–H–C system. The first reactant always includes an S atom, and may include any of the O, H, or C atoms. The second, or the third reactants may include any of the O, H, S, N, or C atoms, and this sequence arranged according to the standard order defines the O–H–S–N–C system.

A number of second and third order reactions includes a second and, respectively, third body M. For these reactions, M will always be placed after all other reactions, e.g.,

$$SO_3 + M \rightarrow SO_2 + O + M,$$
$$\text{or} \quad SO + O + M \rightarrow SO_2 + M.$$

[2] Wagman, D. D., Evans, W. H., Parker, V. B., Halow, I., Bailey, S. M., and Schumm, R. H., "Selected Values of Chemical Thermodynamic Properties," NBS Tech. Note 270-3, pp. 5, 16, 22 (1968).

Most of the chemical reactions included in the table are balanced. There are a number of reactions with unspecified products. In such a case, the word "products" appears after the arrow, e.g., $SO_2 + HO_2 \rightarrow$ products.

Display of Chemical Reactions and Formulae

In order to define the reaction products, the reactants are written using semi-structural formulas. All saturated normal hydrocarbons are written so as to show separately each methyl and methylene group in the chain: CH_4, CH_3CH_3, $CH_3CH_2CH_3$. Unsaturated hydrocarbons are written to show the position of double or triple bonds. The unpaired electron of an alkyl radical is always indicated, with the exception of methyl free radical, e.g.,

Methyl free radical	CH_3 (no dot)
Ethyl, 1-methyl-, free radical (isopropyl)	$(CH_3)_2CH\cdot$
Methyl, hydroxy-, free radical	$\cdot CH_2OH$
Methylthio free radical	$CH_3S\cdot$

If the unpaired electron of an alkyl radical belongs to a carbon in the middle of the chain, it is indicated inside parentheses following the carbon atom, e.g.,

Propyl, 1-methyl-, free radical

(sec-butyl) $CH_3CH_2CH(\cdot)CH_3$

If the oxygen atom of an oxy radical is attached to the terminal carbon atom, the radical is written in the usual manner: CH_3O. If the oxygen atom of the oxy radical is attached to a C atom in the middle of the chain, then the oxygen atom, together with the unpaired electron, are inside parentheses following the C atom: $(CH_3)_2C(O\cdot)CH_2CH_3$. The rules for writing peroxo, and other free radicals are the same as for the oxy free radicals: $CH_3O_2\cdot$, CH_3S.

Atoms like O, H, S, N, C, and simple radicals like OH, HO_2, SH, NH, CH, CH_2, CH_3, CS, CN are written without a dot.

Acknowledgment

This work was supported by the Department of Energy and by the Office of Standard Reference Data of the National Bureau of Standards.

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds

Chemical reactions	n	M	k/k_{ref}	T/K	A	B	E/R (in K)	k factors f	F
$S + O_2 \rightarrow SO + O$									
Sulfur atom + Oxygen molecule									
71 FAI/VAN	2			298	1.7(+12)	–	–	0.9	1.1
72 DAV/KLE1	2			252–423	1.3(+12)	0	0±50	0.8	1.2
72 DON/LIT	2			295	1.0(+12)	–	–	0.8	1.2
75 CLY/TOW	2			298	9.0(+11)	–	–	0.8	1.2
79 CLY/WHI	2			296–410	1.0(+12)	0	−153±108	0.7	1.4
80 BAU/COX (Recommended k).	2			230–400	1.2(+12)	0	0±100	0.7	1.4
k factors apply at 298K only.									
$S + O_3 \rightarrow SO + O_2$									
Sulfur atom + Ozone									
75 CLY/TOW	2			298	7.2(+12)	–	–	0.7	1.3
80 BAU/COX (Recommended k).	2			298	7.2(+12)	–	–	0.5	2.0
$S + H_2 \rightarrow SH + H$									
Sulfur atom + Hydrogen molecule									
76 BAU/DRY (Recommended k).	2			298	1.3(−1)	–	–	0.5	1.5
$k_1 = Kk_{-1}$.									
75 BEN/GOL	2				2.5(+12)	0.5	13640		
Semi–empirical evaluation.									
$S^*(^1D) + H_2 \rightarrow$ products									
Sulfur atom + Hydrogen molecule									
72 LIT/DAL	2		0.22	300	–	–	–		
k_{ref}: $S^*(^1D) + CH_2{=}CH_2 \rightarrow$ products.									
$S + OH \rightarrow SO + H$									
Sulfur atom + Hydroxyl free radical									
75 BEN/GOL	2				6.3(+11)	0.5	0		
Semi–empirical evaluation.									
79 JOU/LEB	2			298	4.0(+13)	–	–	0.8	1.2
$S + OH \rightarrow SH + O$									
Sulfur atom + Hydroxyl free radical									
75 BEN/GOL	2				1.3(+12)	0.5	12700		
Semi–empirical evaluation.									
$S + S + M \rightarrow S_2 + M$									
Sulfur atom									
79 NIC/AMO	3			295	4.3(+18)	–	–	0.8	1.2
$S + S_2 \rightarrow S_2 + S$									
Sulfur atom + Sulfur dimer									
75 BEN/GOL	2				6.3(+11)	0.5	0		
Semi–empirical evaluation.									
$S + SO \rightarrow S_2 + O$									
Sulfur atom + Sulfur monoxide									
75 BEN/GOL	2				6.3(+11)	0.5	11500		
Semi–empirical evaluation.									
$S + SO \rightarrow SO + S$									
Sulfur atom + Sulfur monoxide									
75 BEN/GOL	2				6.3(+11)	0.5	0		
Semi–empirical evaluation.									
$S + SH \rightarrow S_2 + H$									
Sulfur atom + Mercapto free radical									
73 SCH	2			295	2.4(+13)	–	–		
75 BEN/GOL	2				6.3(+11)	0.5	0		
Semi–emprical evaluation.									
79 NIC/AMO	2			295	<3.0(+12)	–	–		
Upper limit k.									

Chemical reactions	n	M	k/k_{ref}	T/K	A	B	E/R (in K)	k factors f	F
$S + SH \rightarrow SH + S$									
Sulfur atom + Mercapto free radical									
75 BEN/GOL	2				6.3(+11)	0.5	4000		
Semi-empirical evaluation.									
$S + N_2 \rightarrow NS + N$									
Sulfur atom + Nitrogen molecule									
75 BEN/GOL	2				4.0(+12)	0.5	55200		
Semi-empirical evaluation.									
$S^*(^1D) + N_2 \rightarrow$ products									
Sulfur atom + Nitrogen molecule									
72/LIT/DAL	2		0.062	300	–	–	–		
k_{ref} : $S^*(^1D) + CH_2{=}CH_2$ + products									
$S + NO \rightarrow SO + N$									
Sulfur atom + Nitrogen oxide(NO)									
75 BEN/GOL	2				4.0(+11)	0.5	17260		
Semi-empirical evaluation.									
$S + NO \rightarrow NS + O$									
Sulfur atom + Nitrogen oxide(NO)									
75 BEN/GOL	2				1.0(+12)	0.5	17365		
Semi-empirical evaluation.									
$S^*(^1D) + NO \rightarrow$ products									
Sulfur atom + Nitrogen oxide(NO)									
72 LIT/DAL	2		0.68		–	–	–		
k_{ref}: $S^*(^1D) + CH_2{=}CH_2 \rightarrow$ products									
$S + NO + M \rightarrow SNO + M$									
Sulfur atom + Nitrogen oxide(NO)									
78 VAN/OBI	2	CO_2		298	9.3(+12)	–	–	0.8	1.2
Limiting high-pressure k.									
78 VAN OBI	3	CO_2		298	1.9(+17)	–	–		
k_0 (low pressure).									
$S + NO_2 \rightarrow SO + NO$									
Sulfur atom + Nitrogen oxide(NO_2)									
75 CLY/TOW	2			298	3.7(+13)	–	–	0.8	1.2
79 CLY/WHY	2			296–410	3.0(+13)	0	–84±60	0.8	1.2
$S^*(^1D) + N_2O \rightarrow NS + NO$									
Sulfur atom + Nitrogen oxide(N_2O)									
72 LIT/DAL	2		0.1	300	–	–	–		
k_{ref}: $S^*(^1D) + CH_2{=}CH_2 \rightarrow$ products									
(Approximate ratio).									
$S + NH \rightarrow SH + N$									
Sulfur atom + Imidogen free radical									
75 BEN/GOL	2				6.3(+11)	0.5	4000		
Semi-empirical evaluation.									
$S^*(^1D) + CO \rightarrow$ products									
Sulfur atom + Carbon monoxide									
72 LIT/DAL	2		0.19	300	–	–	–		
k_{ref}: $S^*(^1D) + CH_2{=}CH_2 \rightarrow$ products									
$S^*(^1D) + CO_2 \rightarrow$ products									
Sulfur atom + Carbon dioxide									
72 LIT/DAL	2		0.24	300	–	–	–		
k_{ref}: $S^*(^1D) + CH_2{=}CH_2 \rightarrow$ products									

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k_{ref}	T/K	A	B	E/R (in K)	k factors f	F
$S^*(^1D) + CH_4 \rightarrow CH_3SH$									
Sulfur atom + Methane									
72 LIT/DAL	2		0.076	300	–	–	–		
k_{ref}: $S^*(^1D) + CH_2{=}CH_2 \rightarrow$ products									
80 ADD/DON	2			295	1.1(+14)	–	–	0.7	1.3
$S + CS \rightarrow CS + S$									
Sulfur atom + Carbon monosulfide free radical									
75 BEN/GOL	2				6.3(+11)	0.5	0		
Semi-empirical evaluation.									
$S + CS \rightarrow S_2 + C$									
Sulfur atom + Carbon monosulfide free radical									
75 BEN/GOL	2				1.6(+12)	0.5	40463		
Semi-empirical evaluation.									
$S + CS + M \rightarrow CS_2 + M$									
Sulfur atom + Carbon monosulfide free radical									
76 BAU/DRY (Recommended k).	3			1800–3700	8.7(+13)	0	–4370	0.5	1.5
$k_1 = Kk_{-1}$.									
$S + CS_2 \rightarrow S_2 + CS$									
Sulfur atom + Carbon disulfide									
76 BAU/DRY (Recommended k).	2			298	3.9(+11)	–	–	0.5	1.5
$S + COS \rightarrow S_2 + CO$									
Sulfur atom + Carbon oxide sulfide									
72 JAK/AHM	2			298	1.1(+10)	–	–		
Evaluation.									
74 KLE/DAV	2			233–245	9.2(+11)	0	1825±60	0.9	1.1
76 BAU/DRY (Recommended k).	2			230–2600	1.7(+12)	0	2050±230	0.3	3.0
$S^*(^1D) + COS \rightarrow S_2 + CO$									
Sulfur atom + Carbon oxide sulfide									
72 LIT/DAL	2		1.5	300	–	–	–	0.7	1.3
k_{ref}: $S^*(^1D) + CH_2{=}CH_2 \rightarrow$ products									
79 ADD/BYR	2			290	7.2(+13)	–	–	0.8	1.3
79 SHE/SAF	2		2.4	298	–	–	–		
k_{ref}: $S^*(^1D) + COS \rightarrow S(^3P) + COS$ (Optimization).									
80 ADD/DON	2			295	1.8(+14)	–	–	0.7	1.3
$S + CN \rightarrow CS + N$									
Sulfur atom + Cyanogen free radical									
75 BEN/GOL	2				6.3(+11)	0.5	0		
Semi-empirical evaluation.									
$S + C_2 \rightarrow CS + C$									
Sulfur atom + Carbon dimer									
75 BEN/GOL	2				6.3(+11)	0.5	0		
Semi-empirical evaluation.									
$S + CH{\equiv}CH \rightarrow$ cy-$CH{=}CHS$									
Sulfur atom + Ethyne									
71 STR/O'C	2			298–450	–	–	–		
k/k_{ref}: $6.2\exp(-1007/T)$.									
k_{ref}: $S + CH_2{=}CH_2 \rightarrow$ cy-CH_2CH_2S									
Conventional photolysis method.									
72 KER/PAR (Recommended k).	2			298	1.7(+11)	–	–		
$S + CH{\equiv}CH \rightarrow$ products									
Sulfur atom + Ethyne									
78 VAN/SAF	2			298–484	3.4(+13)	0	1510±200	0.4	1.6

Chemical reactions	n	M	k/k_{rel}	T/K	A	B	E/R (in K)	k factors f	F
$S + CD{\equiv}CD \rightarrow$ products									
Sulfur atom + Ethyne-d_2									
78 VAN/SAF	2			298	2.3(+11)	–	–	0.8	1.2
$S^*(^1D) + CH_2{=}CH_2 \rightarrow CH_2{=}CHSH$									
Sulfur atom + Ethene									
79 SHE/SAF	2			298	4.2(+13)	–	–		
Optimization.									
$S + CH_2{=}CH_2 \rightarrow$ cy-CH_2CH_2S									
Sulfur atom + Ethene									
71 CON/VAN	2			298	9.0(+11)	–	–	0.9	1.1
Flash photolysis method.									
71 STR/O'C	2		1.0	298–450	–	–	–		
k_{ref}: $S + CH_2{=}CH_2 \rightarrow$ cy-CH_2CH_2S									
Conventional photolysis method.									
72 DAV/KLE2	2			218–442	4.3(+12)	0	795±40	0.9	1.1
72 KER/PAR (Recommended k).	2			298	8.1(+11)	–	–		
$S^*(^1D) + CH_2{=}CH_2 \rightarrow$ cy-$CH_2CH_2S^*$									
Sulfur atom + Ethene									
79 SHE/SAF	2			298	3.8(+13)	–	–		
Optimization.									
$S + CD_2{=}CH_2 \rightarrow$ cy-CD_2CH_2S									
Sulfur atom + Ethene-1,1-d_2									
71 STR/O'C	2		1.07	298–450	–	–	–		
k_{ref}: $S + CH_2{=}CH_2 \rightarrow$ cy-CH_2CH_2S									
Conventional photolysis method.									
$S + cis\text{-}CHD{=}CHD \rightarrow$ cy-CHDCHDS									
Sulfur atom + cis-Ethene-1,2-d_2									
71 STR/O'C	2		1.04	298–450	–	–	–		
k_{ref}: $S + CH_2{=}CH_2 \rightarrow$ cy-CH_2CH_2S									
Conventional photolysis method.									
$S + CD_2{=}CD_2 \rightarrow$ cy-CD_2CD_2S									
Sulfur atom + Ethene-d_4									
71 STR/O'C	2		1.14	298–450	–	–	–		
k_{ref}: $S + CH_2{=}CH_2 \rightarrow$ cy-CH_2CH_2S									
Conventional photolysis method.									
$S^*(^1D) + CH_3CH_3 \rightarrow$ products									
Sulfur atom + Ethane									
72 LIT/DAL	2		0.17	300	–	–	–		
k_{ref}: $S^*(^1D) + CH_2{=}CH_2 \rightarrow$ products									
$S + cy\text{-}CH_2CH_2S \rightarrow S_2 + CH_2{=}CH_2$									
Sulfur atom + Thiirane									
71 STR/O'C	2			298–450	–	–	–		
k/k_{ref}: 8.3exp(+906/T)									
k_{ref}: $S + CH_2{=}CH_2 \rightarrow$ cy-CH_2CH_2S									
Conventional photolysis method.									
73 KLE/DAV1	2			298–355	2.7(+13)	0	0	0.9	1.1
$S + CH_3C{\equiv}CH \rightarrow$ cy-$(CH_3)C{=}CHS$									
Sulfur atom + 1-Propyne									
71 STR/O'C	2			298–450	–	–	–		
k/k_{ref}: 6.2exp(−453/T)									
k_{ref}: $S + CH_2{=}CH_2 \rightarrow$ cy-CH_2CH_2S									
Conventional photolysis method.									
72 KER/PAR (Recommended k).	2			298	1.1(+12)	–	–		
$S + CH_3C{\equiv}CH \rightarrow$ products									
Sulfur atom + Propyne									
78 VAN/SAF	2			298–449	2.0(+13)	0	453±100	0.4	1.6

Chemical reactions	n	M	k/k_{ref}	T/K	A	B	E/R (in K)	k factors f	F
$S + CH_3CH=CH_2 \rightarrow$ cy-$(CH_3)CHCH_2S$									
Sulfur atom + Propene									
71 CON/VAN	2			298	6.0(+12)	–	–	0.8	1.2
Flash photolysis method.									
71 STR/O'C	2			298–450	–	–	–		
k/k_{ref}: 1.0exp(+574/T)									
k_{ref}: $S + CH_2=CH_2 \rightarrow$ cy-CH_2CH_2S									
Conventional photolysis method.									
72 KER/PAR (Recommended k).	2			298	5.8(+12)	–	–		
72 KER/PAR (Recommended ratio).	2		6.9	298	–	–	–		
k_{ref}: $S + CH_2=CH_2 \rightarrow$ cy-CH_2CH_2S									
73 KLE/DAV2	2			214–500	3.6(+12)	0	190±45	0.2	5.2
$S^*(^1D) + CH_3CH=CH_2 \rightarrow$ cy-$(CH_3)CHCH_2S$									
Sulfur atom + Propene									
72 KER/PAR (Recommended ratio).	2		1.7	300	–	–	–		
k_{ref}: $S^*(^1D) + CH_2=CH_2 \rightarrow$ cy-CH_2CH_2S									
$S +$ cy-$(CH_3)CHCH_2S \rightarrow S_2 + CH_3CH=CH_2$									
Sulfur atom + Thiirane,methyl-									
71 STR/O'C	2			298–450	–	–	–		
k/k_{ref}: 8.4exp(+1057/T)									
k_{ref}: $S + CH_2=CH_2 \rightarrow$ cy-CH_2CH_2S									
Conventional photolysis method.									
$S + CH_3CH_2C\equiv CH \rightarrow$ products									
Sulfur atom + 1-Butyne									
78 VAN/SAF	2			298	3.3(+12)	–	–	0.9	1.1
$S + CH_3C\equiv CCH_3 \rightarrow$ cy-$(CH_3)C=C(CH_3)S$									
Sulfur atom + 2-Butyne									
71 STR/O'C	2			298–450	–	–	–		
k/k_{ref}: 2.7exp(+654/T)									
k_{ref}: $S + CH_2=CH_2 \rightarrow$ cy-CH_2CH_2S									
Conventional photolysis method.									
72 KER/PAR (Recommended k).	2			298	1.9(+13)	–	–		
$S + CH_3C\equiv CCH_3 \rightarrow$ products									
Sulfur atom + 2-Butyne									
78 VAN/SAF	2			298	1.6(+13)	–	–	0.9	1.1
$S + CH_2=CHCH=CH_2 \rightarrow$ cy-$(CH_2=CH)CHCH_2S$									
Sulfur atom + 1,3-Butadiene									
71 STR/O'C	2			298–450	–	–	–		
k/k_{ref}: 2.4exp(+1027/T)									
k_{ref}: $S + CH_2=CH_2 \rightarrow$ cy-CH_2CH_2S									
Conventional photolysis method.									
72 KER/PAR (Recomended k).	2			298	6.0(+13)	–	–		
$S + CH_3CH_2CH=CH_2 \rightarrow$ cy-$(CH_3CH_2)CHCH_2S$									
Sulfur atom + 1-Butene									
71 CON/VAN	2			298	9.0(+12)	–	–	0.9	1.1
Flash photolysis method.									
71 STR/O'C	2			298–450	–	–	–		
k/k_{ref}: 0.75exp(+866/T)									
k_{ref}: $S + CH_2=CH_2 \rightarrow$ cy-CH_2CH_2S									
Conventional photolysis method.									
72 KER/PAR	2			298	9.3(+12)	–	–		
72 KER/PAR (Recommended ratio).	2		10.0	298	–	–	–		
k_{ref}: $S + CH_2=CH_2 \rightarrow$ cy-CH_2CH_2S									
73 KLE/DAV2	2			216–475	4.5(+12)	0	180±45	0.1	4.0

Chemical reactions	n	M	k/k_{rel}	T/K	A	B	E/R (in K)	k factors f	F
S + cis-$CH_3CH=CHCH_3$ → cy-$(CH_3)CHCH(CH_3)S$									
Sulfur atom + cis-2-Butene									
71 STR/O'C	2			298–450	–	–	–		
k/k_{rel}: 0.53exp(+1050/T)									
k_{rel}: S + $CH_2=CH_2$ → cy-CH_2CH_2S									
Conventional photolysis method.									
72 KER/PAR (Recommended k).	2			298	1.4(+13)	–	–		
72 KER/PAR (Recommended ratio).	2		16.0	298	–	–	–		
k_{rel}: S + $CH_2=CH_2$ → cy-CH_2CH_2S									
S + cis-$CH_3CH=CHCH_3$ → products									
Sulfur atom + cis-2-Butene									
73 DAV/KLE	2			219–500	2.8(+12)	0	–116±45	0.9	1.1
S + trans-$CH_3CH=CHCH_3$ → cy-$(CH_3)CHCH(CH_3)S$									
Sulfur atom + trans-2-Butene									
71 CON/VAN	2			298	1.2(+13)	–	–	0.8	1.2
Flash photolysis method.									
71 STR/O'C	2			298–450	–	–	–		
k/k_{rel}: 0.65exp(+1010/T)									
k_{rel}: S + $CH_2=CH_2$ → cy-CH_2CH_2S									
Conventional photolysis method.									
72 KER/PAR (Recommended k).	2			298	1.4(+13)	–	–		
72 KER PAR (Recommended ratio).	2		20.0	298	–	–	–		
k_{rel}: S + $CH_2=CH_2$ → cy-CH_2CH_2S									
S + $(CH_3)_2C=CH_2$ → cy-$(CH_3)_2CCH_2S$									
Sulfur atom + 1-Propene, 2-methyl-									
71 CON/VAN	2			298	3.6(+13)	–	–	0.9	1.1
Flash photolysis method.									
71 STR/O'C	2			298–450	–	–	–		
k/k_{rel}: 0.97exp(+1190/T)									
k_{rel}: S + $CH_2=CH_2$ → cy-CH_2CH_2S									
Conventional photolysis method.									
72 KER/PAR (Recommended k).	2			298	4.0(+13)	–	–		
72 KER/PAR (Recommended ratio).	2		50.0	298	–	–	–		
k_{rel}: S + $CH_2=CH_2$ → cy-CH_2CH_2S									
$S^*(^1D)$ + $(CH_3)_2C=CH_2$ → cy-$(CH_3)_2CCH_2S$									
Sulfur atom + 1-Propene, 2-methyl-									
72 KER/PAR (Recommended ratio).	2		3.5	300	–	–	–		
k_{rel}: $S^*(^1D)$ + $CH_2=CH_2$ → cy-CH_2CH_2S									
S + $CH_3CH_2C\equiv CCH_3$ → products									
Sulfur atom + 2-Pentyne									
78 VAN/SAF	2			298	1.8(+13)	–	–	0.8	1.2
S + $CH_3CH_2CH_2CH=CH_2$ → cy-$(CH_3CH_2CH_2)CHCH_2S$									
Sulfur atom + 1-Pentene									
72 KER/PAR (Recommended k).	2			298	8.1(+12)	–	–		
S + $CH_3CH_2C(CH_3)=CH_2$ → cy-$(CH_3CH_2)C(CH_3)CH_2S$									
Sulfur atom + 1-Butene, 2-methyl-									
71 STR/O'C	2			298–450	–	–	–		
k/k_{rel}: 0.78exp(+1424/T)									
k_{rel}: S + $CH_2=CH_2$ → cy-CH_2CH_2S									
Conventional photolysis method.									
72 KER/PAR (Recommended k).	2			298	7.4(+13)	–	–		

Chemical reactions	n	M	k/k_{ref}	T/K	A	B	E/R (in K)	k factors f	F
$S + CH_3CH{=}C(CH_3)_2 \rightarrow$ cy-$(CH_3)CH[C(CH_3)_2]S$									
Sulfur atom + 2-Butene, 2-methyl-									
71 STR/O'C	2			298–450	–	–	–		
k/k_{ref}: 0.51exp(+1515/T)									
k_{ref}: $S + CH_2{=}CH_2 \rightarrow$ cy-CH_2CH_2S									
Conventional photolysis method.									
72 KER/PAR (Recommended k).	2			298	6.5(+13)	–	–		
72 KER/PAR (Recommended ratio).	2		56.0	298	–	–	–		
k_{ref}: $S + CH_2{=}CH_2 \rightarrow$ cy-CH_2CH_2S									
$S + (CH_3)_2C{=}C(CH_3)_2 \rightarrow$ cy-$[(CH_3)_2]CC[(CH_3)_2]S$									
Sulfur atom + 2-Butene, 2,3-dimethyl-									
71 CON/VAN	2			298	>6.2(+13)	–	–	0.9	1.1
Lower limit k.									
Flash photolysis method.									
71 STR/O'C	2			298–450	–	–	–		
k/k_{ref}: 0.50exp(+1690/T)									
k_{ref}: $S + CH_2{=}CH_2 \rightarrow$ cy-CH_2CH_2S									
Conventional photolysis method.									
72 KER/PAR (Recommended k).	2			298	8.5(+13)	–	–		
$S + (CH_3)_2C{=}C(CH_3)_2 \rightarrow$ products									
Sulfur atom + 2-Butene, 2,3-dimethyl-									
73 DAV/KLE	2			252–500	2.8(+12)	0	−650±115	0.6	1.4
$S_2 + O \rightarrow S + SO$									
Sulfur dimer + Oxygen atom									
73 SCH	2			1050	4.2(+12)	–	–		
Approximate k. Given with caution.									
75 BEN/GOL	2				6.3(+11)	0.5	0		
Semi-empirical evaluation.									
$S_2 + H \rightarrow S + SH$									
Sulfur dimer + Hydrogen atom									
75 BEN/GOL	2				7.9(+12)	0.5	8355		
Semi-empirical evaluation.									
$S_2 + S \rightarrow S + S_2$									
Sulfur dimer + Sulfur atom									
75 BEN/GOL	2				6.3(+11)	0.5	0		
Semi-empirical evaluation.									
$S_2 + S_2 + M \rightarrow S_4 + M$									
Sulfur dimer									
72 LAN/OLD	3	CO_2		293	9.1(+17)	–	–	0.1	10.
73 LAN/OLD	3	CO_2		293	3.6(+18)	–	–		
Given with caution.									
79 NIC/AMO	3			295	8.0(+18)	–	–	0.9	1.1
$S_2 + N \rightarrow S + NS$									
Sulfur dimer + Nitrogen atom									
75 BEN/GOL	2				6.3(+11)	0.5	4000		
Semi-empirical evaluation.									
$S_2 + C \rightarrow S + CS$									
Sulfur dimer + Carbon atom									
75 BEN/GOL	2				6.3(+11)	0.5	0		
Semi-empirical evaluation.									
$S_2 + M \rightarrow S + S + M$									
Sulfur dimer									
80 HIG/SAI	2	Ar		4500–6000	4.8(+13)	0	38750		

Chemical reactions	n	M	k/k_{ref}	T/K	A	B	E/R (in K)	k factors f	F
$SO + O \rightarrow O + SO$									
Sulfur monoxide + Oxygen atom									
75 BEN/GOL	2				6.3(+11)	0.5	0		
Semi-empirical evaluation.									
$SO + O \rightarrow S + O_2$									
Sulfur monoxide + Oxygen atom									
75 BEN/GOL	2				2.0(+11)	0.5	2770		
Semi-empirical evaluation.									
$SO + O + M \rightarrow SO_2 + M$									
Sulfur monoxide + Oxygen atom									
71 MIY/TAK1	3	Ar		298	7.3(+16)	–	–	0.9	1.1
76 BAU/DRY (Recommended k).	3			298	6.7(+13)	–	–	0.7	1.3
$SO + O_2 \rightarrow SO_2 + O$									
Sulfur monoxide + Oxygen molecule									
72 BRE/MIL	2			297	<5.0(+7)	–	–		
Upper limit k.									
80 BAU/COX (Recommended k).	2			300–1000	3.6(+11)	0	3300±500	0.3	3.2
k factors apply at 298k only.									
$SO + O_3 \rightarrow SO_2 + O_2$									
Sulfur monoxide + Ozone									
80 BAU/COX (Recommended k).	2			220–300	1.5(+12)	0	1100±400	0.5	2.0
k factors apply at 298K only.									
80 ROB/SMI	2			296	5.2(+10)	–	–	0.8	1.2
$SO + O_3(v=n) \rightarrow SO_2^* + O_2$									
Sulfur monoxide + Ozone									
74 KAL/BRA	2		2.4	300	–	–	–	0.8	1.3
k_{ref}: $SO + O_3 \rightarrow SO_2^* + O_2$									
$SO + H \rightarrow O + SH$									
Sulfur monoxide + Hydrogen atom									
75 BEN/GOL	2				6.3(+11)	0.5	19930		
Semi-empirical evaluation.									
$SO + H \rightarrow S + OH$									
Sulfur monoxide + Hydrogen atom									
75 BEN/GOL	2				4.0(+12)	0.5	11200		
Semi-empirical evaluation.									
$SO + OH \rightarrow SO_2 + H$									
Sulfur monoxide + Hydroxyl free radical									
73 SCH (Recommended k).	2			298	3.3(+13)	–	–	0.5	2.0
79 JOU/LEB	2			298	5.1(+13)	–	–	0.8	1.2
$SO + S \rightarrow O + S_2$									
Sulfur monoxide + Sulfur atom									
75 BEN/GOL	2				6.3(+11)	0.5	11500		
Semi-empirical evaluation.									
$SO + S \rightarrow S + SO$									
Sulfur monoxide + Sulfur atom									
75 BEN/GOL	2				6.3(+11)	0.5	0		
Semi-empirical evaluation.									

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k_{ref}	T/K	A	B	E/R (in K)	k factors f	F
$SO + SO \rightarrow SO_2 + S$									
Sulfur monoxide									
72 BRE/MIL	2			297	<3.0(+10)	–	–		
Upper limit k.									
73 SCH	2			300	<1.8(+9)	–	–		
Upper limit k.									
73 SCH	2			1000	<1.2(+11)	–	–		
Upper limit k.									
75 CHU/CAL	2			298	5.0(+8)	–	–	0.2	1.8
$SO + SO + M \rightarrow (SO)_2 + M$									
Sulfur monoxide									
80 HER/HUI	3			298	1.6(+17)	–	–		
2 – 8 torr.									
$SO + SO_3 \rightarrow SO_2 + SO_2$									
Sulfur monoxide + Sulfur trioxide									
75 CHU/CAL	2			298	1.2(+9)	–	–	0.4	1.6
$SO + (SO)_2 \rightarrow SO_2 + S_2O$									
Sulfur monoxide + Sulfur monoxide dimer									
80 HER/HUI	2			298	2.0(+10)	–	–		
2 – 8 torr.									
$SO + N \rightarrow O + NS$									
Sulfur monoxide + Nitrogen atom									
75 BEN/GOL	2				1.6(+12)	0.5	8254		
Semi-empirical evaluation.									
$SO + N \rightarrow S + NO$									
Sulfur monoxide + Nitrogen atom									
75 BEN/GOL	2				6.3(+11)	0.5	4000		
Semi-empirical evaluation.									
$SO + NO_2 \rightarrow SO_2 + NO$									
Sulfur monoxide + Nitrogen oxide(NO_2)									
71 CUP/GLA	2		1.6	300	–	–	–		
k_{ref}: $O + NO_2 \rightarrow O_2 + NO$									
71 MIY/TAK2	2			298	1.2(+16)	–	–	0.9	1.1
80 BAU/COX (Recommended k).	2			298	8.4(+12)	–	–	0.5	2.0
80 CLY/MAC	2			295	8.2(+12)	–	–	0.9	1.1
$SO + C \rightarrow O + CS$									
Sulfur monoxide + Carbon atom									
75 BEN/GOL	2				6.3(+11)	0.5	0		
Semi-empirical evaluation.									
$SO + C \rightarrow S + CO$									
Sulfur monoxide + Carbon atom									
75 BEN/GOL	2				6.3(+11)	0.5	0		
Semi-empirical evaluation.									
$SO + M \rightarrow S + O + M$									
Sulfur monoxide									
78 AST/GLA	2	Ar		5700–7200	1.6(+14)	0	55330±3610	0.3	4.0
Rate constant expressed as k[Ar].									
$SO_2 + O \rightarrow SO + O_2$									
Sulfur dioxide + Oxygen atom									
76 BAU/DRY (Recommended k).	2			440–2100	1.3(+14)	–0.5	9980	0.3	1.7
$k_1 = Kk_{-1}$.									
80 GRI/REE	2			2630–3570	4.0(+12)	0	9210	0.9	1.1
80 SLA/GRI	2			3500	3.8(+11)	–	–	0.9	1.1

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k_{ref}	T/K	A	B	E/R (in K)	k factors f	F
$SO_2 + O + M \rightarrow SO_3 + M$									
Sulfur dioxide + Oxygen atom									
73 SCH	3			250–1000	3.6(+14)	0	–500	0.5	2.0
M = Ar, O_2, N_2, He.									
k factors are larger at other temperatures.									
74 ATK/PIT3	3	N_2O		299–392	3.3(+16)	0	1000±200		
75 WES/DEH2	3	He		248–415	3.9(+16)	0	1400±50	0.8	1.2
75 WES DEH2	3	He		297	3.0(+14)	–	–	0.9	1.1
M_{eff}: He(1.0)									
75 WES DEH2	3	SO_2		297	2.9(+15)	–	–	0.7	1.3
M_{eff}: SO_2(9.5)									
75 WES DEH2	3	N_2		297	7.2(+14)	–	–	0.9	1.1
M_{eff}: N_2(2.4)									
78 ATK/PIT4	3	Ar		299–400	1.1(+16)	0	1010±150		
78 ATK/PIT4	3	N_2		300	5.0(+14)	–	–	0.8	1.2
78 ATK PIT4	3	SO_2		299	3.4(+15)	–	–	0.7	1.3
79 MER/LEV	3			1685	7.4(+14)	–	–		
80 BAU/COX (Recommended k).	3	N_2		200–400	1.5(+16)	0	1000±200	0.5	2.
k factors apply at 298K only.									
80 BAU/COX (Recommended k).	3	Ar		200–2500	5.4(+28)	–3.75	2650±200	0.5	2.0
k factors apply at 298K only.									
$SO_2 + O_2^*(^1\Delta_g) \rightarrow SO_3 + O$									
Sulfur dioxide + Oxygen molecule									
76 DUM	2			298	1.3(+8)	–	–		
$SO_2^* + O_2 \rightarrow$ products									
Sulfur dioxide + Oxygen molecule									
78 PAR/HEI	2		0.05	298	–	–	–		
k_{ref}: $SO_2^* \rightarrow {}^1SO_2$, or SO_2									
(SO_2^* is a singlet formed on absorption).									
$^1SO_2 + O_2 \rightarrow$ products									
Sulfur dioxide + Oxygen molecule									
78 PAR/HEI	2		0.29	298	–	–	–		
k_{ref}: $^1SO_2 + SO_2 \rightarrow$ products									
($^1SO_2$ is a fluorescent singlet).									
$SO_2^*(^3B_1) + O_2 \rightarrow$ products									
Sulfur dioxide + Oxygen molecule									
78 PAR/HEI	2		0.36	298	–	–	–		
k_{ref}: $SO_2^*(^3B_1) + SO_2 \rightarrow$ products									
$SO_2 + O_3 \rightarrow SO_3 + O_2$									
Sulfur dioxide + Ozone									
74 DAV/PRU	2			300	<6.0(+1)	–	–		
Upper limit k.									
$SO_2 + H + M \rightarrow HSO_2 + M$									
Sulfur dioxide + Hydrogen atom									
76 BAU/DRY (Recommended k).	3			1660–2120	5.1(+15)	–	–	0.5	1.5
$SO_2 + OH \rightarrow$ products									
Sulfur dioxide + Hydroxyl free radical									
80 COX/DER	2			297	4.0(+11)	–	–	0.8	1.2
$SO_2 + OH(v=9) \rightarrow HSO_3$									
Sulfur dioxide + Hydroxyl free radical									
72 WOR/COL	2			298	>1.4(+10)	–	–	0.8	1.2
Lower limit k.									
Unreported T assumed to be 298K.									

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k_{ref}	T/K	A	B	E/R (in K)	k factors f	k factors F
$SO_2 + OH + M \rightarrow HOSO_2 + M$									
Sulfur dioxide + Hydroxyl free radical									
74 COX2	2			294	3.6(+11)	–	–	0.9	1.1
Evaluation.									
Rate constant expressed as k[M]									
with M = $N_2 + O_2$ at 1 atm.									
75 CAS/DAV	2	N_2		298	3.6(+11)	–	–		
Limiting high-pressure k (760 torr).									
75 CAS/DAV	3	N_2		298	5.8(+16)	–	–		
k_o (low pressure: <20 torr).									
75 GOR/MUL1	2	H_2O		435	1.1(+12)	–	–	0.9	1.1
In an atmosphere of water vapor.									
75 HAR/WAY	3	Ar		298	1.6(+17)	–	–	0.7	1.3
75 HAR/WAY	3	N_2		298	2.6(+17)	–	–	0.9	1.1
76 ATK/PER3	2	Ar		298	4.0(+11)	–	–	0.9	1.1
At 760 torr.									
76 ATK/PER3	2	Ar		298	5.0(+11)	–	–		
Limiting high-pressure k.									
76 ATK/PER3	3	Ar		298	5.9(+16)	–	–	0.8	1.2
k_o (low-pressure k).									
77 CAS/TAN	2	N_2		297	3.6(+11)	–	–		
Limiting high-pressure k (760 torr).									
77 CAS/TAN	3	N_2		297	5.8(+16)	–	–		
k_o (low-pressure k).									
77 CAS/TAN	3	N_2		253–297	5.0(+14)	0	–1410		
k_o (low-pressure). On the basis of k_o(297)									
and E_a experimental values.									
77 CAS/TAN	3	N_2		253–297	2.5(+29)	–5.1	0		
k_o (low-pressure k).									
Alternative T-dependent expression.									
79 DAV/RAV	2	N_2		298	5.4(+11)	–	–	0.8	1.3
Total pressure 1 atm. (extrapolated value).									
80 BAU/COX (Recommended k).	3	N_2		200–400	1.7(+24)	–2.9	0	0.5	2.0
k_o (low-pressure k).									
k factors apply at 298K only.									
80 BAU/COX (Recommended k).	2			200–400	1.2(+12)	0	0	0.4	2.5
Limiting high-pressure k.									
k factors apply at 298K only.									
80 HAR/ATK	2	Ar		298–424	7.0(+9)	0	–1193±150	0.7	1.5
Total pressure 650 torr.									
80 HAR/ATK	2	SF_6		298–424	7.6(+10)	0	–753±150	0.7	1.
Total pressure 650 torr.									
80 HAR/ATK	2	N_2		298–424	2.4(+10)	0	–956		
Total pressure 650 torr.									
$SO_2 + HO_2 \rightarrow SO_3 + OH$									
Sulfur dioxide + Hydroperoxyl free radical									
73 PAY/STI	2			300	5.2(+8)	–	–	0.8	1.2
Evaluation.									
74 LLO	2			300	5.2(+8)	–	–	0.9	1.2
Evaluation. Ratio data versus k_{ref}									
for reaction $HO_2 + HO_2 \rightarrow H_2O_2 + O_2$									
79 BUR/CLI				298	<1.2(+7)	–	–		
Upper limit k.									
$SO_2 + HO_2 \rightarrow$ products									
Sulfur dioxide + Hydroperoxyl free radical									
79 GRA/WIN	2			300	<6.0(+5)	–	–		
Upper limit k.									
$SO_2 + HO_2 + M \rightarrow HO_2SO_2 + M$									
Sulfur dioxide + Hydroperoxyl free radical									
79 BUR/CLI	3	He		298	<1.5(+14)	–	–		
Upper limit k.									

Chemical reactions	n	M	k/k_{ref}	T/K	A	B	E/R (in K)	k factors f	k factors F
$SO_2 + SO_2^*(^1B_1) \rightarrow SO^*(^1\Delta_g, ^3\Sigma^-) + SO_3$									
Sulfur dioxide									
75 CHU/CAL	2			298	2.2(+12)	–	–	0.8	1.2
$SO_2 + SO_2^*(^1B_1) \rightarrow SO + SO_3$									
Sulfur dioxide									
78 MAR/REI	2			298	2.0(+14)	–	–		
In an atmosphere of water vapor. (Approximate k).									
$SO_2 + SO_2^*(^3B_1) \rightarrow SO^*(^3\Sigma^-) + SO_3$									
Sulfur dioxide									
75 CHU/CAL	2			298	4.2(+10)	–	–	0.9	1.1
$SO_2 + NO_2 \rightarrow SO_3 + NO$									
Sulfur dioxide + Nitrogen oxide(NO_2)									
71 ARM/CUL	2			703–1193	6.3(+12)	0	13950		
77 FRE/PAL	2			430–1850	6.3(+12)	0	16000		
Extended validity of k reported in 71 ARM/CUL (above), up to 2000K.									
$SO_2 + NO_2^* \rightarrow$ products									
Sulfur dioxide + Nitrogen oxide(NO_2)									
78 IWA/PRE	2			298	8.2(+10)	–	–		
At 50 torr.									
$SO_2 + NO_3 \rightarrow SO_3 + NO_2$									
Sulfur dioxide + Nitrogen oxide(NO_3)									
75 DAU/CAL	2			300	<4.2(+3)	–	–		
Upper limit k.									
$SO_2 + N_2O_5 \rightarrow SO_3 + N_2O_4$									
Sulfur dioxide + Nitrogen oxide(N_2O_5)									
75 DAU/CAL	2			300	<2.5(+1)	–	–		
Upper limit k.									
$^1SO_2^* + CO \rightarrow SO + CO_2$									
Sulfur dioxide + Carbon monoxide									
73 CEH/HEI	2			300	–	–	–		
k_{ref}: $^1SO_2^* + SO_2 \rightarrow$ products. $k/k_{ref} = 5.0 \times 10^{-3}$(at 2537 A")									
73 CEH HEI	2			300	–	–	–		
$k/k_{ref} = 1.5 \times 10^{-3}$(at 3130 A")									
$SO_2^* + CO \rightarrow SO + CO_2$									
Sulfur dioxide + Carbon monoxide									
73 CEH/HEI	2			300	–	–	–		
k_{ref}: $SO_2^* \rightarrow$ products $k/k_{ref} = 2.2 \times 10^{-5}$ (3130 to 3261 A") (SO_2^* is a vibrationally excited singlet).									
$SO_2^{**} + CO \rightarrow SO + CO_2$									
Sulfur dioxide + Carbon monoxide									
73 CEH/HEI	2			300	–	–	–	0.7	1.4
k_{ref}: $SO_2^{**} \rightarrow SO_2$ $k_{ref} = 1.8 \times 10^{-5}$ (2537 to 3261 A") (SO_2^{**} is a chemically active triplet).									
$SO_2 + CO + M \rightarrow$ products									
Sulfur dioxide + Carbon monoxide									
71 BAU/JEF	2	Ar		1770–2453	2.7(+12)	0	24300±600	0.8	1.3
At 27–170 torr pressure.									

Chemical reactions	n	M	k/k_{ref}	T/K	A	B	E/R (in K)	k factors f	F
$SO_2 + CH_3 + M \rightarrow CH_3SO_2 + M$									
Sulfur dioxide + Methyl free radical									
73 JAM/KER	2			298	1.8(+11)	–	–	0.9	1.1
Limiting high-pressure k.									
$SO_2 + CH_3O_2 \cdot \rightarrow CH_3O_2SO_2$									
Sulfur dioxide + Methyldioxy free radical									
79 SAN/SIM	2			298	4.9(+9)	–	–	0.9	1.1
79 SIM/HEI	2		0.0025	296	–	–	–	0.8	1.2
k_{ref}: $NO + CH_3O_2 \cdot \rightarrow NO_2 + CH_3O$									
$SO_2 + CH_3O_2 \rightarrow$ products									
Sulfur dioxide + Methyldioxy free radical									
79 KAN/MCQ	2			296	3.2(+9)	–	–	0.8	1.2
Best k estimate, based on apparent rate constant (k_{app} 2k).									
$SO_2 + CH{\equiv}CH \rightarrow$ products									
Sulfur dioxide + Ethyne									
71 FIF/MOR	2			1550–2150	3.2(+10)	0.5	20535		
Given with caution.									
$SO_2^{**} + CH_2{=}C{=}CH_2 \rightarrow$ products									
Sulfur dioxide + 1,2-Propadiene									
78 PAR/HEI	2		4.0	298	–	–	–		
k_{ref}: $SO_2^{**} + CH_2{=}C{=}CH_2 \rightarrow$ CO + other products									
(SO_2^{**} is a non-emitting triplet).									
$SO_2^*(^3B_1) + cis\text{-}CH_3CH{=}CHCH_3 \rightarrow [cis\text{-}CH_3CH{=}CHCH_3.SO_2]^*$									
Sulfur dioxide + cis-2-Butene									
74 DEM/CAL	2			294	1.3(+14)	–	–	0.9	1.1
$SO_2^*(^3B_1) + trans\text{-}CH_3CH{=}CHCH_3 \rightarrow [trans\text{-}CH_3CH{=}CHCH_3.SO_2]^*$									
Sulfur dioxide + trans-2-Butene									
74 DEM/CAL	2			294	1.2(+14)	–	–	0.9	1.1
$SO_2^*(^1B_1) + (CH_3)_3CH \rightarrow$ products									
Sulfur dioxide + Propane, 2-methyl-									
78 SU /CAL	2			298	8.4(+12)	–	–		
Evaluation.									
$SO_2^*(^3B_1) + (CH_3)_3CH \rightarrow$ products									
Sulfur dioxide + Propane, 2-methyl-									
78 SU /CAL	2			298	8.7(+11)	–	–		
Evaluation.									
$SO_2^*(^3B_1) + cis\text{-}CH_3CH_2CH{=}CHCH_3 \rightarrow [SO_2.CH_3CH_2CH{=}CHCH_3]^*$									
Sulfur dioxide + cis-2-Pentene									
76 WAM	2			295	6.3(+13)	–	–	0.8	1.2
$SO_2^*(^3B_1) + trans\text{-}CH_3CH_2CH{=}CHCH_3 \rightarrow [SO_2.CH_3CH_2CH{=}CHCH_3]^*$									
Sulfur dioxide + trans-2-Pentene									
76 WAM	2			295	1.0(+14)	–	–	0.7	1.3

Chemical reactions	n	M	k/k_{rel}	T/K	A	B	E/R (in K)	k factors f	k factors F
$SO_2 + M \rightarrow SO + O + M$									
Sulfur dioxide									
75 KIE	2	Kr		2900–5200	1.7(+16)	0	56370±2000	0.6	1.6
78 AST/GLA	2	Ar		3700–6500	4.0(+14)	0	53890±2170	0.5	2.0
Rate constant expressed as k[Ar].									
78 JUS/RIM	2	Ar		2500–3400	2.9(+16)	0	58590±2270	0.5	2.2
79 GRI/REE	2	Ar		2800–3880	8.0(+15)	0	54355	0.7	1.3
80 SAI/YOK	2	Ar		4300–6200	3.5(+14)	0	52805		
80 TYA/BAB	2	Ar		4000–6000	3.3(+15)	0	54150		
80 TYA BAB	2	SO_2		4000–6000	5.0(+14)	0	33520		
$SO_3 + O \rightarrow SO_2 + O_2$									
Sulfur trioxide + Oxygen atom									
71 MER/LEV	2			1100–1400	6.5(+14)	0	5435		
k determined in H_2S flame.									
71 MER/LEV	2			900–1600	2.8(+14)	0	6040		
k determined in COS flame.									
72 JAC/WIN	2			300–500	1.5(+8)	0	500		
73 SCH	2			1480–1550	2.8(+14)	0	6040		
Given with caution.									
79 MER/LEV	2			1685	1.5(+11)	–	–		
$SO_3 + O + M \rightarrow SO_2 + O_2 + M$									
Sulfur trioxide + Oxygen atom									
75 WES/DEH1	3	He		298–507	5.0(+16)	0	–785	0.9	1.1
75 WES DEH1	3	He		298	7.3(+17)	–	–	0.9	1.1
M_{eff}: He(1.0)									
75 WES DEH1	3	SO_3		298	<7.3(+18)	–	–		
M_{eff}: SO_3(<10.0). Upper limit ratio.									
75 WES DEH1	3	N_2		298	1.0(+18)	–	–	0.9	1.1
M_{eff}: N_2(1.4)									
$SO_3 + H_2O \rightarrow H_2SO_4$									
Sulfur trioxide + Water									
75 CAS/DAV	2			298	5.5(+11)	–	–	0.8	1.2
$SO_3 + SO \rightarrow SO_2 + SO_2$									
Sulfur trioxide + Sulfur monoxide									
75 CHU/CAL	2			298	1.2(+9)	–	–	0.4	1.6
$SO_3 + N \rightarrow SO_2 + NO$									
Sulfur trioxide + Nitrogen atom									
72 JAC/WIN	2			300	3.0(+8)	–	–		
75 WES/DEH1	2			298	<6.0(+6)	–	–		
Upper limit k.									
$SO_3 + M \rightarrow SO_2 + O + M$									
Sulfur trioxide									
78 AST/GLA	2	Ar		1700–2500	3.2(+15)	0	31880±1320	0.6	1.6
Rate constant expressed as k[Ar].									
79 AST/GLA	2	Ar		1700–2500	3.2(+15)	0	31900±300	0.6	1.6
$S_2O + O \rightarrow SO + SO$									
Sulfur oxide(S_2O) + Oxygen atom									
74 STE/ALV	2			298	9.0(+11)	–	–	0.9	1.1
Evaluation.									
$SH + O \rightarrow S + OH$									
Mercapto free radical + Oxygen atom									
73 SCH	2			298–2500	2.3(+11)	0.67	956		
Theoretical estimate.									
75 BEN/GOL	2				6.3(+11)	0.5	4000		
Semi-empirical evaluation.									

Chemical reactions	n	M	k/k_{ref}	T/K	A	B	E/R (in K)	k factors f	F
$SH + O \rightarrow SO + H$									
Mercapto free radical + Oxygen atom									
75 BEN/GOL	2				6.3(+11)	0.5	0		
Semi-empirical evaluation.									
75 CUP/GLA	2			295	9.6(+13)	–	–	0.7	1.3
$SH + H \rightarrow S + H_2$									
Mercapto free radical + Hydrogen atom									
72 LAN/OLD	2			293	<6.0(+12)	–	–		
73 BRA/TRU	2			298	2.5(+13)	–	–		
75 CUP/GLA	2			298	1.5(+13)	–	–	0.7	1.3
76 BAU/DRY (Recommended k).	2			298	1.5(+13)	–	–	0.5	1.5
79 NIC/AMO	2			295	1.3(+13)	–	–	0.8	1.2
$SH + H \rightarrow H + SH$									
Mercapto free radical + Hydrogen atom									
75 BEN/GOL	2				6.3(+11)	0.5	0		
Semi-empirical evaluation.									
$SH + S \rightarrow H + S_2$									
Mercapto free radical + Sulfur atom									
73 SCH	2			295	2.4(+13)	–	–		
75 BEN/GOL	2				6.3(+11)	0.5	0		
Semi-empirical evaluation									
79 NIC/AMO	2			295	<3.0(+12)	–	–		
Upper limit k.									
$SH + S \rightarrow S + SH$									
Mercapto free radical + Sulfur atom									
75 BEN/GOL	2				6.3(+11)	0.5	4000		
Semi-empirical evaluation.									
$SH + SH \rightarrow H_2 + S_2$									
Mercapto free radical									
73 SCH	2			295	<3.0(+10)	–	–		
Estimated upper limit k.									
$SH + SH \rightarrow H_2S + S$									
Mercapto free radical									
72 LAN/OLD	2			293	<1.8(+13)	–	–		
Upper limit k.									
73 BRA/TRU	2			298	7.8(+12)	–	–		
76 BAU/DRY (Recommended k).	2			295	7.8(+12)	–	–	0.5	1.5
79 NIC/AMO	2			295	1.9(+13)	–	–	0.9	1.1
$SH + N \rightarrow H + NS$									
Mercapto free radical + Nitrogen atom									
75 BEN/GOL	2				6.3(+11)	0.5	403		
Semi-empirical evaluation.									
$SH + N \rightarrow S + NH$									
Mercapto free radical + Nitrogen atom									
75 BEN/GOL	2				6.3(+11)	0.5	9060		
Semi-empirical evaluation.									
$SH + NO \rightarrow$ products									
Mercapto free radical + Nitrogen oxide(NO)									
73 BRA/TRU	2			298	6.3(+11)	–	–		
$SH + C \rightarrow H + CS$									
Mercapto free radical + Carbon atom									
75 BEN/GOL	2				6.3(+11)	0.5	0		
Semi-empirical evaluation.									

Chemical reactions	n	M	k/k_{rel}	T/K	A	B	E/R (in K)	k factors f	k factors F
$SH + C \rightarrow S + CH$									
Mercapto free radical + Carbon atom									
75 BEN/GOL	2				4.0(+11)	0.5	6090		
Semi-empirical evaluation.									
$H_2S + O \rightarrow SH + OH$									
Hydrogen sulfide + Oxygen ntom									
73 SCH	2			200–350	3.8(+11)	0	920±45	0.5	2.0
76 WHY/TIM	2			263–495	4.4(+12)	0	1660±50	0.9	1.1
78 WHY/TIM	2			263–495	4.4(+12)	0	1660±50	0.8	1.2
80 BAU/COX (Recommended k).	2			250–500	4.3(+12)	0	1660±150	0.8	1.3
k factors apply at 298K only.									
$D_2S + O \rightarrow SD + OD$									
Hydrogen sulfide(D_2S) + Oxygen atom									
76 WHY/TIM	2			298–450	6.3(+12)	0	2145±155	0.5	1.5
$H_2S + O \rightarrow$ products									
Hydrogen sulfide + Oxygen atom									
78 SLA/BAL	2			281–497	1.5(+13)	0	1920±45	0.8	1.2
k based on editor's least square fit of 6 given experimental points.									
79 SIN/IRW	2			297–502	1.6(+13)	0	2171±202	0.5	1.5
$H_2S + O_3 \rightarrow SO_2 + H_2O$									
Hydrogen sulfide + Ozone									
75 BEC/INO	2			298	<1.2(+4)	–	–		
Upper limit k.									
Unreported T assumed to be 298K.									
75 GLA/TOB1	2			293–343	4.9(+10)	0	3420		
Estimated k.									
75 GLA/TOB2	2			298–343	1.6(+12)	0	2620±600	0.2	6.3
75 BAU/DRY (Recommended k).	2			298	4.0(+2)	–	–	0.1	10.0
$H_2S + H \rightarrow SH + H_2$									
Hydrogen sulfide + Hydrogen atom									
71 KUR/PET	2			190–464	7.8(+12)	0	860±30	0.9	1.1
72 ROM/SCH	2			298	2.3(+11)	–	–	0.8	1.3
73 BRA/TRU	2			298	5.0(+11)	–	–		
76 BAU/DRY (Recommended k).	2			190–470	7.8(+12)	0	860±50	0.5	1.5
79 NIC/AMO	2			295	5.0(+11)	–	–	0.9	1.1
80 HUS/SLA	2			300	5.2(+11)	–	–	0.9	1.1
$D_2S + D \rightarrow SD + D_2$									
Hydrogen sulfide(D_2S) + Deuterium atom									
80 HUS/SLA	2			300	4.8(+11)	–	–	0.9	1.1
$H_2S + OH \rightarrow SH + H_2O$									
Hydrogen sulfide + Hydroxyl free radicnl									
73 WES/DEH3	2			298–885	1.4(+13)	0	443		
74 STU	2			298	1.9(+12)	–	–	0.8	1.2
76 BAU/DRY (Recommended k).	2			298–900	6.3(+12)	0	200±150	0.7	1.3
k factors changing to: f = 0.5 and F = 1.5 at 900K.									
76 PER/ATK1	2			297–427	3.1(+12)	0	0	0.9	1.1
80 BAU/COX (Recommended k).	2			250–400	6.6(+12)	0	225±225	0.8	1.3
k factors apply at 298K only.									
$H_2S + OH \rightarrow$ products (overall)									
Hydrogen sulfide + Hydroxyl free rndicnl									
72 NIK/MOR1	2			300	5.2(+12)	–	–		
Approximate k.									
80 COX/SHE	2			297	3.0(+12)	–	–	0.9	1.1

Chemical reactions	n	M	k/k_{ref}	T/K	A	B	E/R (in K)	k factors f	F
$H_2S + OH(v=9) \rightarrow$ products									
Hydrogen sulfide + Hydroxyl free radical									
72 WOR/COL	2			298	>1.5(+11)	–	–	0.6	1.4
Lower limit k.									
Unreported T assumed to be 298K.									
$H_2S + CH_3 \rightarrow SH + CH_4$									
Hydrogen sulfide + Methyl free radical									
76 KER/PAR	2			300–600	2.0(+11)	0	2065±150	0.4	2.5
Tentative k value.									
$H_2S + M \rightarrow SH + H + M$									
Hydrogen sulfide									
76 HIG/SAI	2	Ar		2380–3000	1.3(+16)	0	46300		
77 BOW/DOD	2	Ar		2700–3800	2.0(+13)	0	37300±960	0.7	1.5
$CS + O \rightarrow S + CO$									
Carbon monosulfide free radical + Oxygen atom									
71 HAN/SMI	2			298	8.4(+12)	–	–		
Evaluation.									
73 SCH	2			298	8.4(+12)	–	–	0.5	2.0
Approximate k.									
73 SCH	2			900	9.0(+13)	–	–	0.5	2.0
Approximate k.									
75 BEN/GOL	2				6.3(+11)	0.5	0		
Semi-empirical evaluation.									
77 LIL/RIC	2			150–300	1.6(+14)	0	760±140	0.8	1.2
78 KOL	2			300	1.3(+13)	–	–	0.8	1.2
Unreported T assumed to be 300K.									
80 BAU/COX (Recommended k).	2			150–300	1.6(+14)	0	760±250	0.8	1.3
k factors apply at 298K only.									
$CS + O \rightarrow S + CO(v=n)$									
Carbon monosulfide free radical + Oxygen atom									
72 HAN/RID	2		0.1	298	–	–	–		
k_{ref}: $CS + O \rightarrow S + CO(v=13)$									
Ratio increasing from 0.1 to 0.9 between v=7 and v=12, then decreasing to 0.3 from v=14 to v=15.									
Unreported T assumed to be 298K.									
75 SLA/GRA1	2			305	1.2(+13)	–	–	0.9	1.1
76 BID/BRE	2			300	1.4(+13)	–	–	0.8	1.2
$CS + O \rightarrow SO + C$									
Carbon monosulfide free radical + Oxygen atom									
75 BEN/GOL	2				1.6(+12)	0.5	28940		
Semi-empirical evaluation.									
$CS + O_2 \rightarrow SO + CO$									
Carbon monosulfide free radical + Oxygen molecule									
73 SCH	2			298	<1.8(+6)	–	–		
Estimated upper limit k.									
$CS + O_2 \rightarrow COS + O$									
Carbon monosulfide free radical + Oxygen molecule									
73 SCH	2			298	<1.8(+6)	–	–		
Estimated upper limit k.									
$CS + H \rightarrow S + CH$									
Cnrbon monosulfide free radical + Hydrogen atom									
75 BEN/GOL	2				1.3(+13)	0.5	50930		
Semi-empirical evaluation.									

Chemical reactions	n	M	k/k_{ref}	T/K	A	B	E/R (in K)	k factors f	F
$CS + H \rightarrow SH + C$									
Carbon monosulfide free radical + Hydrogen atom									
75 BEN/GOL	2				2.0(+13)	0.5	48870		
Semi-empirical evaluation.									
$CS + S \rightarrow S + CS$									
Carbon monosulfide free radical + Sulfur atom									
75 BEN/GOL	2				6.3(+11)	0.5	0		
Semi-empirical evaluation.									
$CS + S \rightarrow C + S_2$									
Carbon monosulfide free radical + Sulfur atom									
75 BEN/GOL	2				1.6(+12)	0.5	40463		
Semi-empirical evaluation.									
$CS + S + M \rightarrow CS_2 + M$									
Carbon monosulfide free radical + Sulfur atom									
76 BAU/DRY (Recommended k).	3			1800–3700	8.7(+13)	0	–4370	0.5	1.5
$k_1 = Kk_{-1}$									
$CS + N \rightarrow S + CN$									
Carbon monosulfide free radical + Nitrogen atom									
75 BEN/GOL	2				1.3(+12)	0.5	1160		
Semi-empirical evaluation.									
$CS + N \rightarrow C + NS$									
Carbon monosulfide free radical + Nitrogen atom									
75 BEN/GOL	2				4.0(+12)	0.5	37200		
Semi-empirical evaluation.									
$CS + C \rightarrow S + C_2$									
Carbon monosulfide free radical + Carbon atom									
75 BEN/GOL	2				5.0(+11)	0.5	20435		
Semi-empirical evaluation.									
$CS + C \rightarrow C + CS$									
Carbon monosulfide free radical + Carbon atom									
75 BEN/GOL	2				6.3(+11)	0.5	0		
Semi-empirical evaluation.									
$CS_2 + O \rightarrow CO + S_2$									
Carbon disulfide + Oxygen atom									
79 HSU/SHA	2			298	3.5(+10)	–	–	0.9	1.1
$CS_2 + O \rightarrow CS + SO$									
Carbon disulfide + Oxygen atom									
71 TAK	2			298	1.4(+12)	–	–	0.9	1.1
75 WEI/TIM	2			218–293	1.7(+13)	0	645±35	0.9	1.1
76 BAU/DRY (Recommended k).	2			200–1000	2.2(+13)	0	700	0.7	1.3
$CS_2 + O \rightarrow COS + S$									
Carbon disulfide + Oxygen atom									
73 SCH	2			1100	1.2(+12)	–	–		
Approximate k.									
74 SLA/GIL	2		0.093	302	–	–	–		
k_{ref}: $CS_2 + O \rightarrow$ products									
76 BAU/DRY (Recommended k).	2			302	2.2(+11)	–	–	0.5	1.5
77 GRA/GUT	2		0.098	249–500	–	–	–		
k_{ref}: $CS_2 + O \rightarrow$ products within the given T range, the k/k_{ref} ratio decreases from 0.098±0.004 at 249K to 0.081±0.007 at 500K.									

Chemical reactions	n	M	k/k_{ref}	T/K	A	B	E/R (in K)	k factors f	k factors F
$CS_2 + O \rightarrow COS + S$ —continued									
77 GRA GUT	2			249–500	1.7(+11)	–	–	0.9	1.2
Within the given T range, k increases from $1.7x10^{11}$ at 249K to $5.5x10^{11}cm^3mol^{-1}s^{-1}$ at 500K.									
$CS_2 + O \rightarrow$ products									
Carbon disulfide + Oxygen atom									
74 SLA/GIL	2			302	2.4(+12)	–	–		
74 GRA/GUT	2			249–500	1.7(+12)	–	–	0.9	1.1
Non-linear Arrhenius behavior. Within the given T range, k increases from $1.7x10^{12}$ at 249K to $6.7x10^{12}cm^3mol^{-1}s^{-1}$ at 500K.									
80 BAU/COX (Recommended k).	2			200–500	3.5(+13)	0	700±100	0.6	1.6
k factors apply at 298K only.									
$CS_2 + OH \rightarrow$ products									
Carbon disulfide + Hydroxyl free radical									
78 ATK/PER1	2			300	<4.2(+10)	–	–		
Upper limit k.									
78 ATK PER1	2			425	<6.0(+10)	–	–		
Upper limit k.									
78 KUR2	2			296	1.1(+11)	–	–	0.8	1.2
80 BAU/COX (Recommended k).	2			298	<1.2(+11)	–	–		5.0
Upper limit k.									
80 COX/SHE	2			297	2.6(+11)	–	–	0.7	1.3
80 IYE/ROW	2			298	<1.8(+9)	–	–		
Upper limit k.									
80 WIN/SHA	2			251	<6.0(+9)	–	–		
Upper limit k.									
80 WIN SHA	2			297	<9.0(+8)	–	–		
Upper limit k.									
80 WIN SHA	2			363	<9.6(+8)	–	–		
Upper limit k.									
$CS_2 + S \rightarrow CS + S_2$									
Carbon disulfide + Sulfur atom									
76 BAU/DRY (Recommended k).	2			298	3.9(+11)	–	–	0.5	1.5
$CS_2 + M \rightarrow CS + S + M$									
Carbon disulfide									
76 BAU/DRY (Recommended k).	2	Ar		1800–3700	2.6(+15)	0	38960±9000	0.5	1.5
80 SAI/TOR	2	Ar		2000–2900	2.5(+14)	0	37240		
$CS_2 + M \rightarrow$ products									
Carbon disulfide									
74 TRA	2				6.8(+14)	0	36000±700		
k measured in shock tube. Unspecified high T range.									
$COS + O \rightarrow SO + CO$									
Carbon oxide sulfide + Oxygen ntom									
71 KRE	2			300–523	9.8(+12)	0	2265		
71 KRE/SIM	2			300–523	9.8(+12)	0	2265		
72 BRE/MIL	2			297	7.2(+9)	–	–	0.8	1.2
74 KLE/STI	2			263–502	9.9(+12)	0	2167±28	0.9	1.1
75 WEI/TIM	2			239–404	1.2(+13)	0	2150±35	0.8	1.2
76 MAN/BRA (Recommended k).	2			296	8.4(+9)	–	–	0.9	1.1
k factors changing to: f = 0.3 and F = 3.0 above 300K.									
78 YOS/SAI	2			298	7.1(+9)	–	–	0.9	1.1
80 BAU/COX (Recommended k).	2			220–600	1.6(+13)	0	2250±150	0.6	1.6
k factors apply at 298K only.									
80 ROB/SMI	2			296	1.0(+10)	–	–	0.9	1.1

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k_{ref}	T/K	A	B	E/R (in K)	k factors f	F
$COS + O^*(^1D) \rightarrow SO + CO$									
Carbon oxide sulfide + Oxygen atom									
75 GAU/SNE	2		4.1	300	–	–	–		
k_{ref}: $O_2 + O^*(^1D) \rightarrow O_2^*(^1\Sigma_g^+) + O$									
75 GAU SNE	2			300	1.8(+14)	–	–		
Evaluation.									
$COS + H \rightarrow CO + SH$									
Carbon oxide sulfide + Hydrogen atom									
72 ROM/SCH	2			298	1.3(+10)	–	–	0.8	1.3
75 TSU/YOK	2			300–525	9.1(+12)	0	1965±185	0.9	1.1
76 BAU/DRY (Recommended k).	2			298	1.3(+10)	–	–	0.8	1.3
76 LEE	2			298–478	9.8(+13)	0	2775±40	0.9	1.1
77 LEE/STI	2			261–500	5.5(+12)	0	1940±55	0.8	1.2
$COS + OH \rightarrow$ products									
Carbon oxide sulfide + Hydroxyl free radical									
78 ATK/PER1	2			299	<4.2(+9)	–	–		
Upper limit k.									
78 ATK PER1	2			430	<1.2(+10)	–	–		
Upper limit k.									
78 KUR2	2			296	3.4(+10)	–	–		
80 BAU/COX (Recommended k).	2			298	<3.6(+10)	–	–		5.0
Upper limit k.									
80 COX/SHE	2			297	<2.4(+10)	–	–		
Upper limit k.									
$COS + OH(v=9) \rightarrow$ products									
Carbon oxide sulfide + Hydroxyl free radical									
72 WOR/COL	2			298	1.5(+10)	–	–	0.4	1.6
Unreported T assumed to be 298K.									
$COS + S \rightarrow CO + S_2$									
Carbon oxide sulfide + Sulfur atom									
72 JAK/AHM	2			298	1.1(+10)	–	–		
Evaluation.									
74 KLE/DAV	2			233–245	9.2(+11)	0	1825±60	0.9	1.1
76 BAU/DRY (Recommended k).	2			230–2600	1.7(+12)	0	2050±230	0.3	3.0
$COS + S^*(^1D) \rightarrow CO + S_2$									
Carbon oxide sulfide + Sulfur atom									
72 LIT/DAL	2		1.5	300	–	–	–		
k_{ref}: $CH_2=CH_2 + S^*(^1D) \rightarrow$ products									
78 SHE/SAF	2		2.4	298	–	–	–		
k_{ref}: $COS + S^*(^1D) \rightarrow COS + S(^3P)$									
Optimization.									
79 ADD/BYR	2			290	7.2(+13)	–	–	0.8	1.3
80 ADD/DON	2			295	1.8(+14)	–	–	0.7	1.3
$COS + CD_3 \rightarrow CO + CD_3S$									
Carbon oxide sulfide + Methyl-d_3 free radical									
72 JAK/AHM	2			354–490	3.8(+11)	0	5710±175	0.6	1.8
Evaluation.									
$COS + CN \rightarrow SCN + CO$									
Carbon oxide sulfide + Cyanogen free radical									
79 ADD/LEI	2			295	>1.8(+13)	–	–		
Lower limit k.									
$COS + M \rightarrow$ products									
Carbon oxide sulfide									
74 TRA	2				8.3(+14)	0	31700±650		
k measured in shock tube.									
Unspecified, high T range.									

Chemical reactions	n	M	k/k_{ref}	T/K	A	B	E/R (in K)	k factors f	F
$CH_3S + CH{\equiv}CH \rightarrow CH_3SCH{=}CH$									
Methylthio free radical + Ethyne									
72 KER/PAR (Recommended k).	2			298–333	7.9(+7)	–	–		
$CH_3S + CH_2{=}CH_2 \rightarrow CH_3SCH_2CH_2$									
Methylthio free radical + Ethene									
72 KER/PAR (Recommended k).	2			298	4.8(+8)	–	–		
$CH_3S + cy\text{-}CH_2CH_2S \rightarrow CH_3S_2 + CH_2{=}CH_2$									
Methylthio free radical + Thiirane									
72 JAK/AHM Approximate k.	2			304–478	3.2(+11)	0	4430		
$CH_3S + CH_3CH{=}CHCH_3 \rightarrow CH_3CH(SCH_3)CH(\cdot)CH_3$									
Methylthio free radical + 2-Butene									
72 KER/PAR cis–trans equilibrium–weighted k.	2			298–333	1.6(+9)	–	–		
$CH_3SH \rightarrow CH_3 + SH$									
Methanethiol									
70 BEN/O'N Critical evaluation.	1			1005–1102	3.2(+15)	0	38550		
$CH_3SH + O \rightarrow$ products									
Methanethiol + Oxygen atom									
76 SLA/GRA	2			300	1.1(+12)	–	–		
78 KIR/VET	2			300–661	8.5(+12)	0	–625±36	0.9	1.1
78 SLA/BAL Non–linear Arrhenius behavior. Within the given T range, k increasing from 1.1×10^{12} at 254K to 2.6×10^{12} $cm^3mol^{-1}s^{-1}$ at 495K.	2			254–495	1.1(+12)	–	–		
$CH_3SH + OH \rightarrow$ products									
Methanethiol + Hydroxyl free radical									
80 COX/SHE	2			297	5.4(+13)	–	–	0.9	1.1
$CH_3SH + CH_3 \rightarrow CH_2SH + CH_4$									
Methanethiol + Methyl free radical									
76 KER/PAR (Recommended k).	2			303	1.2(+8)	–	–	0.5	2.0
$CD_3SH + CH_3 \rightarrow CD_3S + CH_4$									
Methane–d_3–thiol + Methyl free radical									
76 KER/PAR (Recommended k).	2			400–500	1.1(+11)	0	2065±500	0.5	2.0
$CD_3SH + CH_3 \rightarrow CD_2SH + CH_3D$									
Methane–d_3–thiol + Methyl free radical									
76 KER/PAR (Recommended k).	2			400–500	7.6(+10)	0	4200±250	0.5	2.0
76 KER/PAR (Recommended k).	2			400–500	1.1(+11)	0	2065±500	0.5	2.0
$CD_3SH + CH_3 \rightarrow CD_2SH + CH_3D$									
Methane–d_3–thiol + Methyl free radical									
76 KER/PAR (Recommended k).	2			400–500	7.6(+10)	0	4200±250	0.5	2.0
$cy\text{-}CH_2CH_2S^* \rightarrow CH_2{=}CHSH$									
Thiirane									
79 SHE/SAF	1			298	5.0(+10)	–	–		
$cy\text{-}CH_2CH_2S + O \rightarrow CH_2{=}CH_2 + SO$									
Thiirane + Oxygen atom									
76 LEE/TIM	2			268–424	8.1(+12)	0	18±20	0.9	1.1

Chemical reactions	n	M	k/k_{rel}	T/K	A	B	E/R (in K)	k factors f	F
cy-CH_2CH_2S + O_3 → CH_2=CH_2 + other products									
Thiirane + Ozone									
80 MAR/HER	2			296	<1.0(+4)	–	–		
8 torr. pressure.									
cy-CH_2CH_2S + H → CH_2=CH_2 + SH									
Thiirane + Hydrogen atom									
75 YOK/AHM	2			300–425	5.7(+13)	0	978±88	0.9	1.1
cy-CH_2SCH_2 + H → cy-CH_2SCH + H_2									
Thiirane + Hydrogen atom									
76 LEE	2			298	7.1(+11)	–	–	0.8	1.2
cy-CH_2CH_2S + S → CH_2=CH_2 + S_2									
Thiirane + Sulfur atom									
71 STR/O'C	2			298–450	–	–	–		
k/k_{rel}: 8.3exp(+906/T)									
k_{rel}: CH_2=CH_2 + S → cy-CH_2CH_2S									
Conventional photolysis method.									
73 KLE/DAV1	2			298–355	2.7(+13)	0	0	0.9	1.1
cy-CH_2CH_2S + CH_3 → CH_2=CH_2 + CH_3S									
Thiirane + Methyl free radical									
72 JAK/AHM	2			304–478	7.1(+10)	0	3370±400	0.3	3.3
cy-CH_2CH_2S + CD_3 → CH_2=CH_2 + CD_3S									
Thiirane + Methyl-d_3 free radical									
72 JAK/AHM	2			303–477	5.9(+10)	0	3270±500	0.2	4.4
Evaluation.									
cy-CH_2CH_2S + CD_3 → cy-$CH_2CH(\,)S$ + CD_3H									
Thiirane + Methyl-d_3 free radical									
72 JAK/AHM	2			303–477	2.2(+11)	0	4800±500	0.3	4.0
Evaluation.									
76 KER/PAR (Recommended k).	2			300–500	2.2(+11)	0	4800±500	0.5	2.0
cy-CH_2CH_2S + CH_3S → CH_2=CH_2 + CH_3S_2									
Thiirane + Methylthio free radical									
72 JAK/AHM	2			304–478	3.2(+11)	0	4430		
Approximate k.									
CH_3SCH_2 + CH_4 → $(CH_3)_2S$ + CH_3									
Methyl, (methylthio)–, free radical + Methane									
76 ART/LEE	2			393–518	6.3(+11)	0	7662		
Evaluation based on k_{-1} and thermodynamic data.									
CH_3CH_2SH → CH_2=CH_2 + H_2S									
Ethanethiol									
70 BEN/O'N	1			785–938	1.0(+13)	0	25900		
Critical evaluation.									
CH_3CH_2SH → CH_3CH_2 + SH									
Ethanethiol									
70 BEN/O'N	1			785–938	6.3(+15)	0	36336		
Critical evaluation.									
CH_3CH_2SH + O → products									
Ethanethiol + Oxygen atom									
76 SLA/GRA	2			300	1.7(+12)	–	–		
78 KIR/VET	2			304–421	5.8(+12)	0	–391±18	0.9	1.1
78 SLA/BLA	2			257–495	1.9(+12)	–	–		
Non-linear Arrhenius behavior. Within the given T range, k increasing from 1.9×10^{12} at 257K to 3.2×10^{12} $cm^3mol^{-1}s^{-1}$ at 495K.									

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k_{ref}	T/K	A	B	E/R (in K)	k factors f	F
$CH_3CH_2SH + CH_3 \rightarrow$ products									
Ethanethiol + Methyl free radical									
76 KER/PAR	2			303	3.5(+7)	–	–	0.5	2.0
Tentative k.									
$(CH_3)_2S + O \rightarrow CH_3S(O) + CH_3$									
Methane, thiobis–, + Oxygen atom									
76 LEE/TIM	2			268–424	8.6(+12)	0	–366±16	0.9	1.1
76 SLA/GRA	2			300	3.8(+13)	–	–		
78 SLA/BAL	2			252–493	3.8(+13)	–	–		
Possible non–linear Arrhenius behavior. Within the given T range, k decreasing from 3.8×10^{13} at 252K to 2.2×10^{13} $cm^3 mol^{-1} s^{-1}$ at 493K.									
80 LEE/TAN1	2			272–472	7.7(+12)	0	–404±30	0.9	1.1
$(CH_3)_2S + O \rightarrow$ products									
Methune,thiobis–, + Oxygen atom									
74 CAD/WIC	2			300	3.3(+11)	–	–		
$(CH_3)_2S + O_3 \rightarrow$ products									
Methane, thiobis–, + Ozone									
78 MAR/HER	2			296	<5.0(+5)	–	–		
Upper limit k.									
$(CH_3)_2S + H \rightarrow CH_3SH + CH_3$									
Methane, thiobis–, + Hydrogen atom									
79 YOK/STR	2			300–472	1.7(+13)	0	1320±44	0.8	1.2
80 YOK/STR	2			300–472	1.7(+13)	0	1319±44	0.8	1.2
Indirect measurement.									
$(CH_3)_2S + H \rightarrow CH_3SCH_2 + H_2$									
Methune, thiobis–, + Hydrogen atom									
76 LEE	2			300	9.0(+10)	–	–	0.7	1.3
$(CH_3)_2S + OH \rightarrow$ products									
Methane, thiobis–, + Hydroxyl free radical									
78 ATK/PER1	2			300	5.9(+12)	–	–	0.9	1.1
78 ATK PER1	2			299–430	3.3(+12)	0	–179±150		
78 KUR1 (Recommended k).	2			273–426	3.7(+12)	0	134±135	0.6	1.4
80 COX/SHE	2			297	5.5(+12)	–	–	0.8	1.2
$(CH_3)_2S + CH_3 \rightarrow CH_3SCH_2 + CH_4$									
Methane, thiobis–, + Methyl free radical									
76 ART/LEE	2			393–518	4.2(+11)	0	4613±82	0.8	1.2
$CH_3SSCH_3 + O \rightarrow$ products									
Disulfide, dimethyl–, + Oxygen atom									
80 LEE/TAN2	2			270–329	1.3(+14)	0	0	0.9	1.1
$CH_3SSCH_3 + H \rightarrow CH_3S + CH_3SH$									
Disulfide, dimethyl–, + Hydrogen atom									
80 EKW/JOD	2			298–428	5.7(+12)	0	–50±50	0.8	1.2
$CH_3SSCH_3 + OH \rightarrow$ products									
Disulfide, dimethyl–, + Hydroxyl free radical									
80 COX/SHE	2			297	1.3(+14)	–	–	0.6	1.4
$CH_3SO_2CH_3 \rightarrow CH_3SO_2 + CH_3$									
Methane, sulfonylbis–									
70 BEN/O'N	1			783–913	2.0(+14)	0	30500		
Critical evaluation.									

Chemical reactions	n	M	k/k_{ref}	T/K	A	B	E/R (in K)	k factors f	F
cy-$CH_2CH_2CH_2S$ + CH_3 → cy-$CH_2CH(\cdot)CH_2S$ + CH_4									
Thietane + Methyl free radical									
76 KER/PAR	2			300–450	3.2(+11)	0	4630±750		
Tentative k.									
cy-$(CH_3)CHCH_2S$ + S → $CH_3CH{=}CH_2$ + S_2									
Thiirane, methyl-, + Sulfur atom									
71 STR/O'C	2			298–450	–	–	–		
k/k_{ref}: 8.4exp(+1057/T)									
k_{ref}: $CH_2{=}CH_2$ + S → cy-CH_2CH_2S									
Conventional photolysis method.									
cy-$(CH_3)CHCH_2S$ + CH_3 → $CH_3CH{=}CH_2$ + CH_3S									
Thiirane, methyl-, + Methyl free radical									
72 JAK/AHM	2			339–435	2.1(+11)	0	3750±830	0.1	8.3
Evaluation.									
cy-$(CH_3)CHCH_2S$ + CH_3 → cy-$[(CH_2)CHCH_2]S$ + CH_4									
Thiirane, methyl-, + Methyl free radical									
72 JAK/AHM	2			339–435	1.0(+11)	0	4160±440	0.3	3.0
$CH_3CH_2CH_2SH$ + O → products									
1-Propanethiol + Oxygen atom									
78 KIR/VET	2			303–421	8.3(+12)	0	–494±22	0.9	1.1
$(CH_3)_2CHSH$ + CH_3 → products									
2-Propanethiol + Methyl free radical									
76 KER/PAR	2			303	4.1(+7)	–	–		
Tentative k.									
cy-$CH_2CH_2CH_2CH_2S$ + H → $CH_2CH_2CH_2CH_2SH$									
Thiophene, tetrahydro-, + Hydrogen atom									
78 HOR/NIS	2			295–576	8.5(+12)	0	1010		
At 5 torr.									
$CH_3C(S)SCH_2CH_3$ → CH_4 + CS_2 + $CH_2{=}CH_2$									
Ethane(dithioic) acid ethyl ester									
78 ALA/BIG	1			629	1.8(−3)	–	–		
78 ALA BIG	1			651–716	9.2(+12)	0	22730		
k based on reported $\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$.									
$CH_3CH_2CH_2CH_2SH$ + O → products									
1-Butanethiol + Oxygen atom									
78 KIR/VET	2			306–419	5.8(+12)	0	–321±19	0.9	1.1
$CH_3CH_2CH_2CH_2SH$ + H → $CH_3CH_2CH_2CH_2$ + H_2S									
1-Butanethiol + Hydrogen atom									
78 HOR/NIS	2			295–576	1.6(+12)	0	1120		
At 5 torr.									
$CH_3CH_2CH_2CH_2SH$ + H → $CH_3CH_2CH_2CH_2S$ + H_2									
1-Butanethiol + Hydrogen atom									
78 HOR/NIS	2			295–576	1.3(+13)	0	1600		
At 5 torr.									
$(CH_3)_3CSH$ → $(CH_3)_2C{=}CH_2$ + H_2S									
2-Propanethiol, 2-methyl-									
70 BEN/O'N	1			950–1230	2.5(+13)	0	27830		
Critical evaluation.									
$(CH_3)_3CSH$ + CH_3 → $(CH_3)_3CS$ + $CH_2C(CH_3)_2SH$ + CH_4									
2-Propanethiol, 2-methyl-, + Methyl free radical									
76 KER/PAR	2			303	5.9(+7)	–	–		
Tentative k.									

Chemical reactions	n	M	k/k_{ref}	T/K	A	B	E/R (in K)	k factors f	F
$CH_2{=}CHCH_2SO_2CH_3 \rightarrow CH_2{=}CHCH_2 + CH_3SO_2$									
1-Propene, 3-methylsulfonyl-									
70 BEN/O'N	1			573–633	5.0(+12)	0	28030		
Critical evaluation.									
$CH_3SC(O)OCH_2CH_3 \rightarrow CH_3SH + CO_2 + CH_2{=}CH_2$									
Carbonothioic acid O-ethyl S-methyl ester									
79 ALA/BIG	1			629	1.0(−4)	–	–		
79 ALA BIG	1			490–550	1.8(+12)	0	23500		
k based on reported $\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$.									
$CH_3OC(O)SCH_2CH_3 \rightarrow CH_3OH + COS + CH_2{=}CH_2$									
Carbonothioic acid S-ethyl O-methyl ester									
79 ALA/BIG	1			629	7.8(−7)	–	–		
79 ALA BIG	1			490–550	1.2(+13)	0	27800		
k based on reported $\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$.									
$CH_3CH_2CH_2CH_2CH_2SH + O \rightarrow$ products									
1-Pentonethiol + Oxygen ntom									
78 KIR/VET	2			302–409	6.2(+12)	0	−328±19	0.9	1.1
$CH_3OC(O)SCH(CH_3)_2 \rightarrow CH_3OH + COS + CH_3CH{=}CH_2$									
Carbonothioic acid O-methyl S-(1-methylethyl) ester									
79 ALA/BIG	1			629	4.6(−5)	–	–		
79 ALA BIG	1			440–480	8.4(+12)	0	25000		
k based on reported $\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$.									
$CH_3SC(O)OCH(CH_3)_2 \rightarrow CH_3SH + CO_2 + CH_3CH{=}CH_2$									
Carbonothioic acid S-methyl O-(1-methylethyl) ester									
79 ALA/BIG	1			629	9.4(−3)	–	–		
79 ALA BIG	1			547–584	6.7(+11)	0	20060		
k based on reported $\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$. (Evacuated sealed tube method).									
$CH_3SC(O)OC(CH_3)_3 \rightarrow CH_3SHH + CO_2 + CH_2{=}C(CH_3)_2$									
Carbonothioic acid O-(1,1-dimethylethyl) S-methyl ester									
79 ALA/BIG	1			629	4.2(−1)	–	–		
79 ALA BIG	1			479–502	5.4(+10)	0	16080		
k based on reported $\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$. (Inhibited sealed tube method).									
$CH_3OC(O)SC(CH_3)_3 \rightarrow CH_3OH + COS + CH_2{=}C(CH_3)_2$									
Carbonothioic acid S-(1,1-dimethylethyl) O-methyl ester									
79 ALA/BIG	1			629	1.2(−3)	–	–		
79 ALA BIG	1			370–420	1.4(+12)	0	21800		
k based on reported $\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$.									
$CH_3C(S)SCH_2CH_2CH_2CH_3 \rightarrow$ $CH_4 + CS_2 + CH_2{=}CHCH_2CH_3$									
Ethane(dithioic) acid butyl ester									
78 ALA/BIG	1			629	3.3(−3)	–	–		
78 ALA BIG	1			651–716	1.2(+13)	0	22500		
k based on reported $\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$.									
$CH_3C(S)SCH(CH_3)CH_2CH_3 \rightarrow$ $CH_4 + CS_2 + CH_2{=}CHCH_2CH_3$ + cis-, and trans-$CH_3CH{=}CHCH_3$									
Ethane(dithioic) acid 1-methylpropyl ester									
78 ALA/BIG	1			629	7.4(−2)	–	–		
78 ALA BIG	1			584–639	6.7(+12)	0	20210		
k based on reported $\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$.									

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k_{ref}	T/K	A	B	E/R (in K)	k factors f	F
$CH_3C(S)SC(CH_3)_3 \rightarrow CH_4 + CS_2 + (CH_3)_2C{=}CH_2$									
Ethanet(dithioic) acid 1,1–dimethylethyl ester									
78 ALA/BIG	1			629	3.1(−1)	–	–		
78 ALA BIG	1			448–502	1.1(+13)	0	19600		
k based on reported $\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$									
$(CH_3)_3CSC(CH_3)_3 \rightarrow (CH_3)_2{=}CH_2 + H_2S + (CH_3)_3SH + (CH_3)_3SH$									
Propane, 2,2'–thiobis[2–methyl–									
80 MAR/BAR	1			633–686	1.3(+15)	0	27545±962	0.5	2.0
$(CH_3)_3CSSC(CH_3)_3 \rightarrow (CH_3)_2C{=}CH_2$ + other products									
Disulfide, bis(1,1–dimethylethyl)–									
76 MAR/BAR	1			603–673	4.0(+14)	0	22130±480	0.4	2.5
In a stirred–flow system.									
76 MAR BAR	1			519–573	4.0(+13)	0	21290±240	0.6	1.6
In a static system.									

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Appendix: Conversion Tables

Equivalent second order rate constants

A \ B	cm^3 mol^{-1} s^{-1}	dm^3 mol^{-1} s^{-1}	m^3 mol^{-1} s^{-1}	cm^3 $molecule^{-1}$ s^{-1}	$(mm\ Hg)^{-1}$ s^{-1}	atm^{-1} s^{-1}	ppm^{-1} min^{-1}	m^2 kN^{-1} s^{-1}
1 cm^3 mol^{-1} s^{-1} =	1	10^{-3}	10^{-6}	1.66×10^{-24}	$1.604 \times 10^{-5}\ T^{-1}$	$1.219 \times 10^{-2}\ T^{-1}$	2.453×10^{-9}	$1.203 \times 10^{-4}\ T^{-1}$
1 dm^3 mol^{-1} s^{-1} =	10^3	1	10^{-3}	1.66×10^{-21}	$1.604 \times 10^{-2}\ T^{-1}$	$12.19\ T^{-1}$	2.453×10^{-6}	$1.203 \times 10^{-1} T^{-1}$
1 m^3 mol^{-1} s^{-1} =	10^6	10^3	1	1.66×10^{-18}	$16.04\ T^{-1}$	$1.219 \times 10^4\ T^{-1}$	2.453×10^{-3}	$120.3\ T^{-1}$
1 cm^3 $molecule^{-1}$ s^{-1} =	6.023×10^{23}	6.023×10^{20}	6.023×10^{17}	1	$9.658 \times 10^{18}\ T^{-1}$	$7.34 \times 10^{21}\ T^{-1}$	1.478×10^{15}	$7.244 \times 10^{19}\ T^{-1}$
1 $(mm\ Hg)^{-1}$ s^{-1} =	$6.236 \times 10^4\ T$	$62.36\ T$	$6.236 \times 10^{-2}\ T$	$1.035 \times 10^{-19}\ T$	1	760	4.56×10^{-2}	7.500
1 atm^{-1} s^{-1}	$82.06\ T$	$8.206 \times 10^{-2}\ T$	$8.206 \times 10^{-5}\ T$	$1.362 \times 10^{-22}\ T$	1.316×10^{-3}	1	6×10^{-5}	9.869×10^{-3}
1 ppm^{-1} min^{-1} = at 298 K, 1 atm total pressure	4.077×10^8	4.077×10^5	407.7	6.76×10^{-16}	21.93	1.667×10^4	1	164.5
1 m^2 kN^{-1} s^{-1} =	$8314\ T$	$8.314\ T$	$8.314 \times 10^{-3}\ T$	$1.38 \times 10^{-20}\ T$	0.1333	101.325	6.079×10^{-3}	1

To convert a rate constant from one set of units A to a new set B find the conversion factor for the row A under column B and multiply the old value by it, e.g. to convert cm^3 $molecule^{-1}$ s^{-1} to m^3 mol^{-1} s^{-1} multiply by 6.023×10^{17}.

Table adapted from High Temperature Reaction Rate Data No. 5, The University, Leeds (1970).

Equivalent third order rate constants

A \ B	cm^6 mol^{-2} s^{-1}	dm^6 mol^{-2} s^{-1}	m^6 mol^{-2} s^{-1}	cm^6 $molecule^{-2}$ s^{-1}	$(mm\ Hg)^{-2}$ s^{-1}	atm^{-2} s^{-1}	ppm^{-2} min^{-1}	m^4 kN^{-2} s^{-1}
1 cm^6 mol^{-2} s^{-1} =	1	10^{-6}	10^{-12}	2.76×10^{-46}	$2.57 \times 10^{-10}\ T^{-2}$	$1.48 \times 10^{-4}\ T^{-2}$	1.003×10^{-19}	$1.447 \times 10^{-6}\ T^{-2}$
1 dm^6 mol^{-2} s^{-1} =	10^6	1	10^{-6}	2.76×10^{-42}	$2.57 \times 10^{-4}\ T^{-2}$	$148\ T^{-2}$	1.003×10^{-13}	$1.447 \times 10^{-2}\ T^{-2}$
1 m^6 mol^{-2} s^{-1} =	10^{12}	10^6	1	2.76×10^{-36}	$257\ T^{-2}$	$1.48 \times 10^8\ T^{-2}$	1.003×10^{-7}	$1.447 \times 10^4\ T^{-2}$
1 cm^6 $molecule^{-2}$ s^{-1} =	3.628×10^{47}	3.628×10^{41}	3.628×10^{35}	1	$9.328 \times 10^{37}\ T^{-2}$	$5.388 \times 10^{43}\ T^{-2}$	3.64×10^{26}	$5.248 \times 10^{39}\ T^{-2}$
1 $(mm\ Hg)^{-2}$ s^{-1} =	$3.89 \times 10^9\ T^2$	$3.89 \times 10^3\ T^2$	$3.89 \times 10^{-3}\ T^2$	$1.07 \times 10^{-38}\ T^2$	1	5.776×10^5	3.46×10^{-5}	56.25
1 atm^{-2} s^{-1} =	$6.733 \times 10^3\ T^2$	$6.733 \times 10^{-3}\ T^2$	$6.733 \times 10^{-9}\ T^2$	$1.86 \times 10^{-44}\ T^2$	1.73×10^{-6}	1	6×10^{-11}	9.74×10^{-5}
1 ppm^{-2} min^{-1} = at 298 K, 1 atm total pressure	9.97×10^{18}	9.97×10^{12}	9.97×10^6	2.75×10^{-29}	2.89×10^4	1.667×10^{10}	1	1.623×10^6
1 m^4 kN^{-2} s^{-1} =	$6.91 \times 10^7\ T^2$	$69.1\ T^2$	$6.91 \times 10^{-5}\ T^2$	$1.904 \times 10^{-40}\ T^2$	0.0178	1.027×10^4	6.16×10^{-7}	1

See note to table for second order rate constants.

NBS-114A (REV. 2-80)

U.S. DEPT. OF COMM. BIBLIOGRAPHIC DATA SHEET (See instructions)	1. PUBLICATION OR REPORT NO. NSRDS-NBS 72	2. Performing Organ. Report No.	3. Publication Date May 1982

4. TITLE AND SUBTITLE

Tables of Rate Constants for Gas Phase Chemical Reactions of Sulfur Compounds (1971-1980)

5. AUTHOR(S) Francis Westley

6. PERFORMING ORGANIZATION (If joint or other than NBS, see instructions)

NATIONAL BUREAU OF STANDARDS
DEPARTMENT OF COMMERCE
WASHINGTON, D.C. 20234

7. Contract/Grant No.

8. Type of Report & Period Covered N/A

9. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS (Street, City, State, ZIP)

Morgantown Energy Technology Center
Department of Energy
Morgantown, WV 26505

and Office of Standard Reference Data
National Bureau of Standards
Washington, DC 20234

10. SUPPLEMENTARY NOTES

Library of Congress Catalog Card Number: 82-2094

☐ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

11. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)

A table of rate constants for gas phase chemical reactions of sulfur compounds is presented. Specifically, it gives in tabular form the values of the parameters for the modified Arrhenius equation $k = AT^B \exp(-E/RT)$. The table covers the reactions of sulfur containing molecules and free radicals, S, S_2, SO, SO_2, SO_3, S_2O, SH, H_2S, CS, CS_2, COS, $CH_3S\cdot$, CH_3SH, cy-CH_2CH_2S, $CH_3SCH_2\cdot$ and a number of thiols, thioethers, and thioesters, with other compounds. The table includes 19 unimolecular, 208 bimolecular, and 13 termolecular reactions totaling 240 distinct chemical reactions. There are 441 rate constants associated with these reactions, distributed as follows: 30 for first order reactions, 377 for second order reactions, and 34 for third order reactions. The kinetic data were compiled from 145 experimental papers and 8 critical reviews published between 1971 and 1980.

12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)

Arrhenius parameters; chemical kinetics; combustion; decomposition; free radicals; gas phase; hydrocarbons; hydrogen; nitrogen; oxygen; rate of reaction; sulfur

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